LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019898.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.123	3	6	15	rVB	2705515	3016099	91.74%	9.406%
2	3.746	107	112	120	rBV2	45843	87516	2.66%	0.273%
3	3.864	128	132	136	rBV	49508	60545	1.84%	0.189%
4	3.993	150	154	160	rVB2	26888	42372	1.29%	0.132%
5	4.064	160	166	177	rVB	189285	318199	9.68%	0.992%
6	4.240	191	196	202	rBV	66163	95080	2.89%	0.297%
7	4.305	202	207	213	rBV2	78532	125002	3.80%	0.390%
8	4.452	228	232	240	rVB	77227	108861	3.31%	0.339%
9	4.587	247	255	258	rBV2	28234	49301	1.50%	0.154%
10	4.634	258	263	268	rVV	352572	517202	15.73%	1.613%
11	4.687	268	272	284	rVB2	197551	357966	10.89%	1.116%
12	4.852	296	300	303	rBV2	21710	33480	1.02%	0.104%
13	5.017	322	328	338	rBV	287457	427337	13.00%	1.333%
14	5.470	398	405	421	rBV	1210292	1848443	56.23%	5.764%
15	5.793	449	460	465	rBV2	53005	93672	2.85%	0.292%
16	6.099	503	512	516	rBV	30381	74238	2.26%	0.232%
17	6.205	526	530	543	rVB3	45438	94541	2.88%	0.295%
18	6.752	614	623	647	rVB4	160268	540455	16.44%	1.685%
19	7.069	670	677	684	rBV	1266076	2113631	64.29%	6.592%
20	7.122	684	686	692	rVB2	29770	39652	1.21%	0.124%
21	7.293	706	715	730	rBV2	122399	366707	11.15%	1.144%
22	7.516	749	753	761	rVB2	21373	35952	1.09%	0.112%
23	7.599	761	767	774	rBV2	68627	129730	3.95%	0.405%
24	7.893	812	817	825	rVB	358289	574869	17.49%	1.793%
25	8.058	839	845	850	rBV	28513	47497	1.44%	0.148%
26	8.140	853	859	863	rVV2	47147	90705	2.76%	0.283%
27	8.187	863	867	872	rVV6	17779	37006	1.13%	0.115%
28	8.869	972	983	988	rBV4	29368	82427	2.51%	0.257%
29	8.922	988	992	998	rVB6	17345	37963	1.15%	0.118%
30	9.069	1009	1017	1033	rBV	825060	1479200	44.99%	4.613%
31	9.352	1056	1065	1070	rBV8	17419	51827	1.58%	0.162%
32	9.816	1137	1144	1152	rBV3	36894	97132	2.95%	0.303%
33	10.057	1179	1185	1192	rBV5	31726	68544	2.08%	0.214%
34	10.187	1198	1207	1222	rVB9	18873	68206	2.07%	0.213%
35	10.563	1264	1271	1276	rVB	31850	51748	1.57%	0.161%
36	10.699	1285	1294	1311	rVB	466468	828630	25.21%	2.584%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.893	1317	1327	1342	rBV3	27124	78662	2.39%	0.245%
38	11.087	1352	1360	1366	rBV7	31168	96265	2.93%	0.300%
39	11.140	1366	1369	1374	rVB	25122	39366	1.20%	0.123%
40	11.346	1399	1404	1406	rBV2	30270	44948	1.37%	0.140%
41	11.381	1406	1410	1415	rVV	40529	67724	2.06%	0.211%
42	11.452	1416	1422	1429	rVV3	52411	111168	3.38%	0.347%
43	11.534	1429	1436	1443	rVB2	29763	64774	1.97%	0.202%
44	12.587	1608	1615	1628	rVB4	30983	64152	1.95%	0.200%
45	12.922	1662	1672	1675	rBV5	20611	41138	1.25%	0.128%
46	13.163	1703	1713	1732	rBV	1740427	2698611	82.09%	8.416%
47	13.446	1752	1761	1773	rBV	1293212	2126035	64.67%	6.630%
48	14.540	1940	1947	1958	rVB	761842	1158836	35.25%	3.614%
49	14.763	1976	1985	1999	rVB	270851	648384	19.72%	2.022%
50	16.034	2192	2201	2219	rBV	1538197	2361167	71.82%	7.363%
51	17.298	2410	2416	2430	rBV	950618	1473420	44.82%	4.595%
52	17.981	2527	2532	2540	rBV4	21617	37652	1.15%	0.117%
53	18.198	2563	2569	2587	rBV	320763	512631	15.59%	1.599%
54	19.116	2722	2725	2738	rVB7	39324	53624	1.63%	0.167%
55	19.339	2760	2763	2771	rVB3	46809	63174	1.92%	0.197%
56	19.433	2775	2779	2789	rVV	108802	163400	4.97%	0.510%
57	19.869	2848	2853	2861	rBV	2721585	3287485	100.00%	10.252%
58	20.880	3022	3025	3028	rVB	61587	65449	1.99%	0.204%
59	21.128	3063	3067	3076	rBV3	130276	179366	5.46%	0.559%
60	21.398	3108	3113	3123	rBV	1036404	1424980	43.35%	4.444%
61	23.821	3519	3525	3536	rVB	526237	1111857	33.82%	3.467%

Sum of corrected areas: 32066003

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
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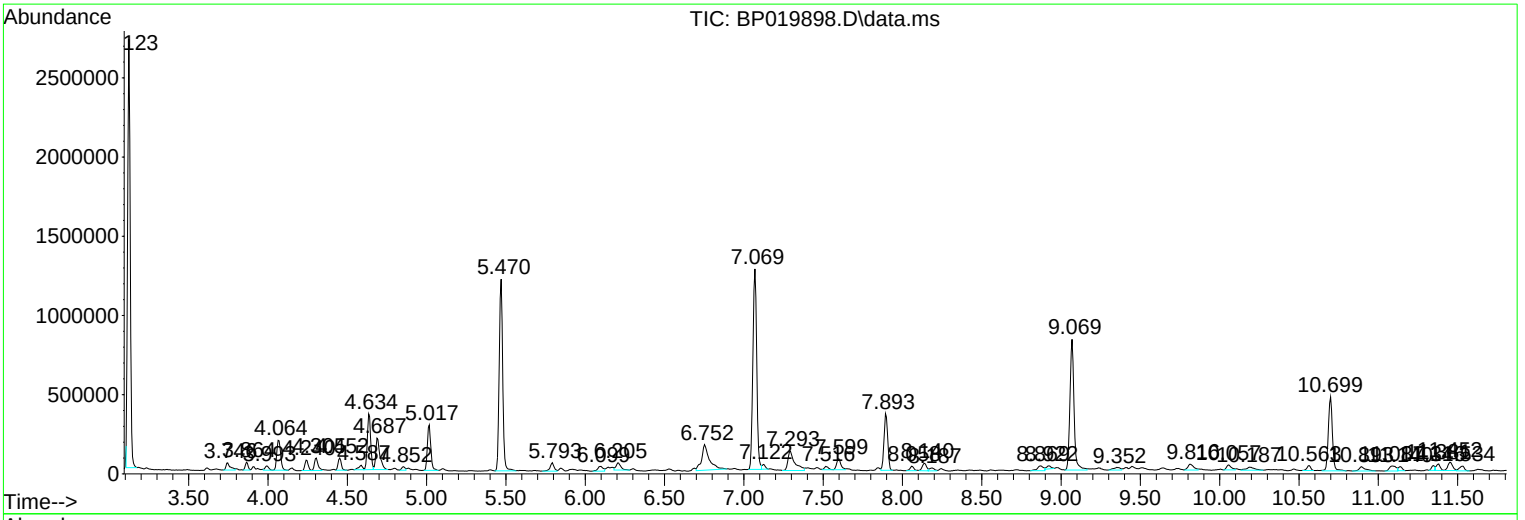
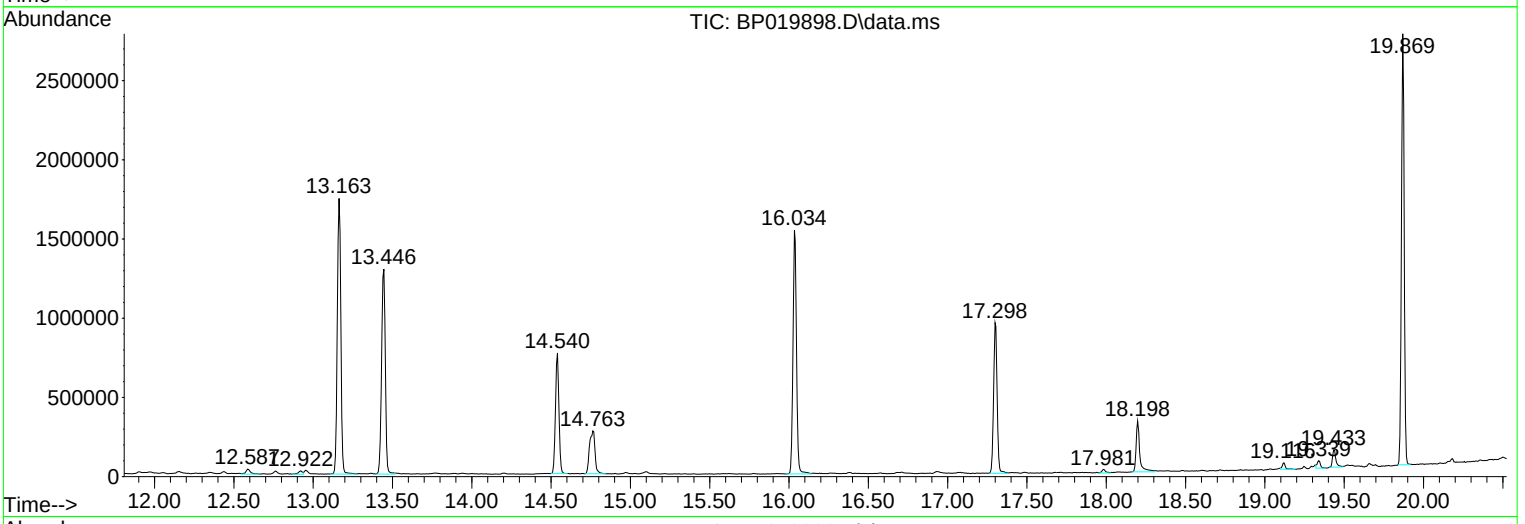
Misc :
ALS Vial : 13 Sample Multiplier: 1

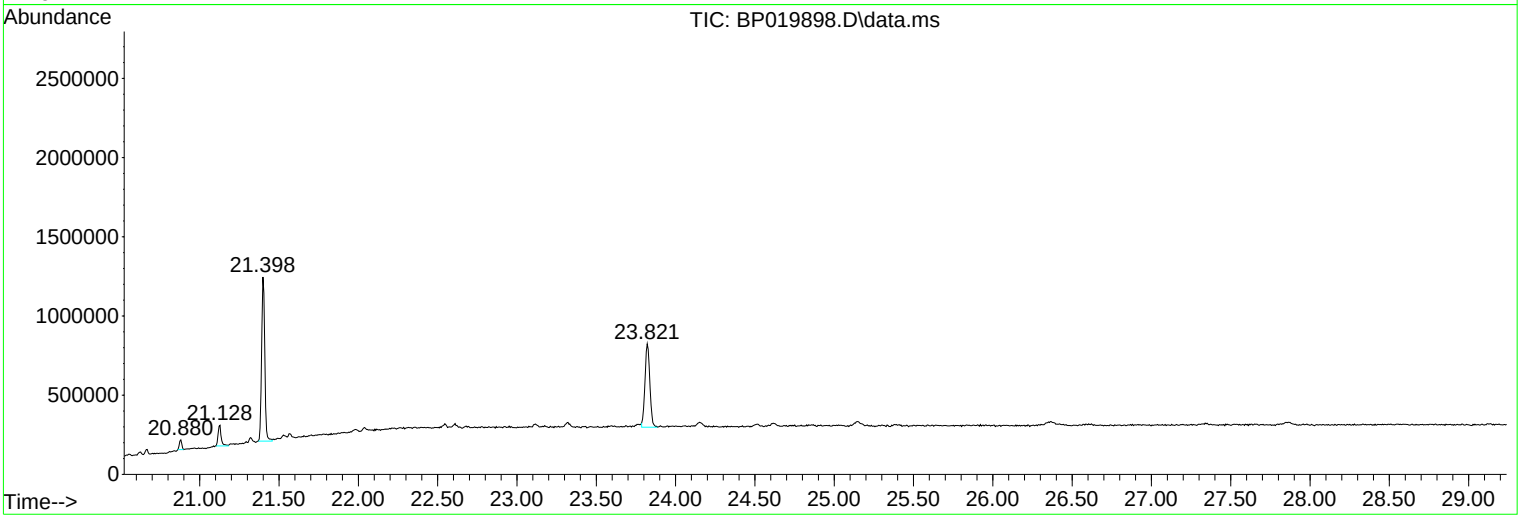
Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

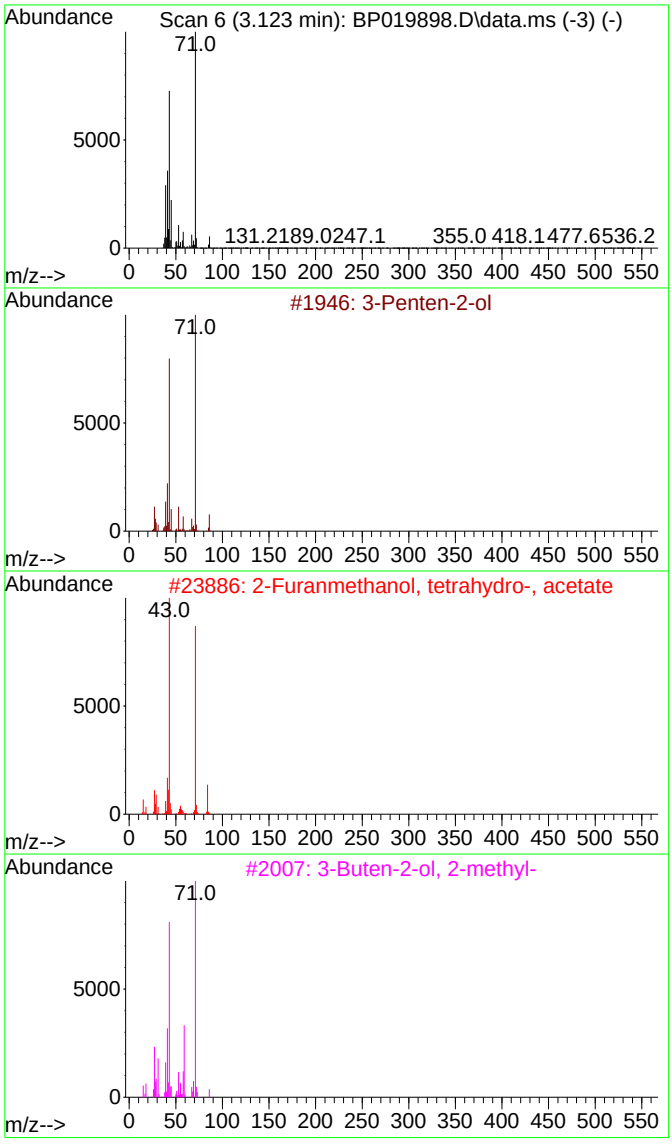
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

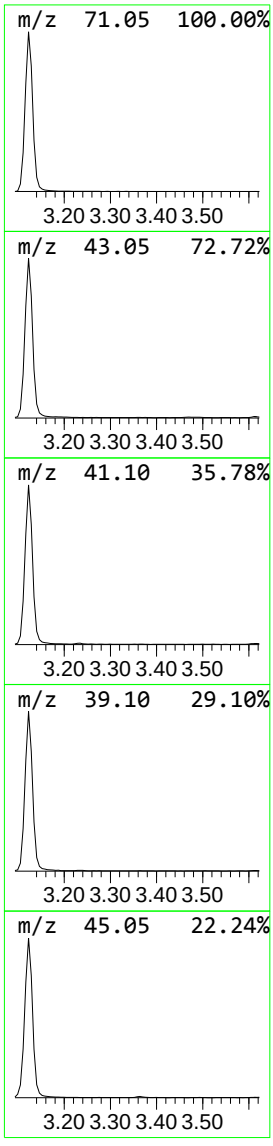
****

Peak Number 1 3-Penten-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.123	104.93 ng	3016100	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	80
2	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	45
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	45
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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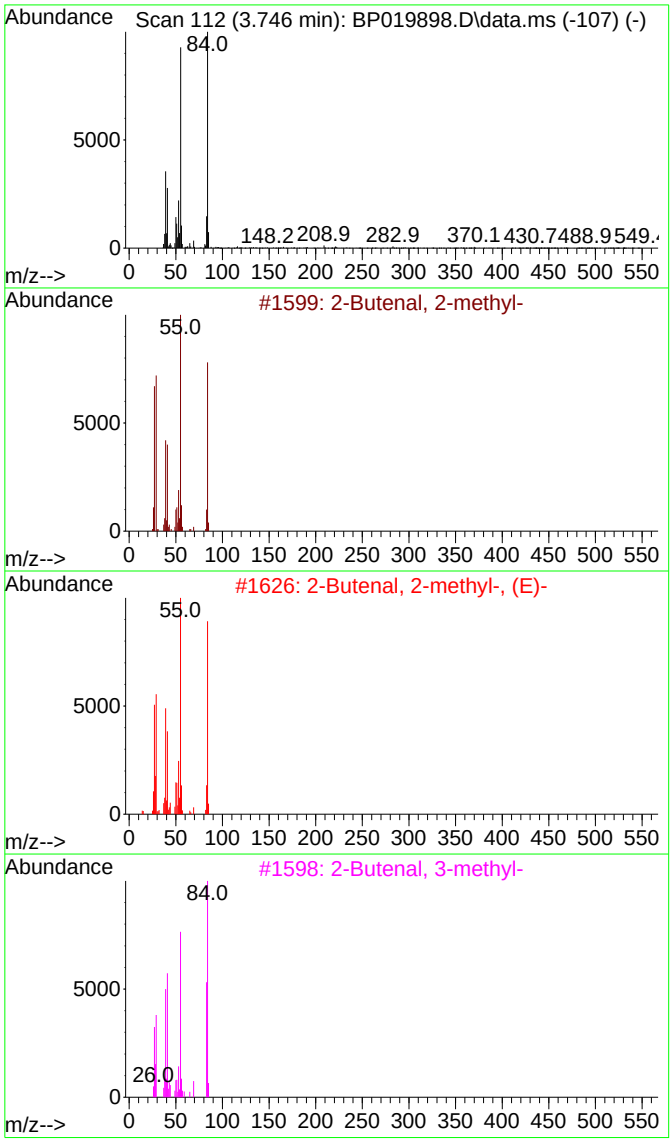
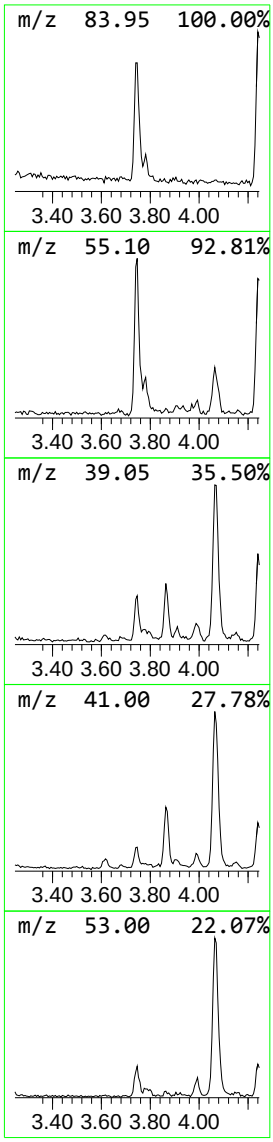
Peak Number 2 2-Butenal, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.746	3.04 ng	87516	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	91
2	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	91
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	87
4	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	56
5	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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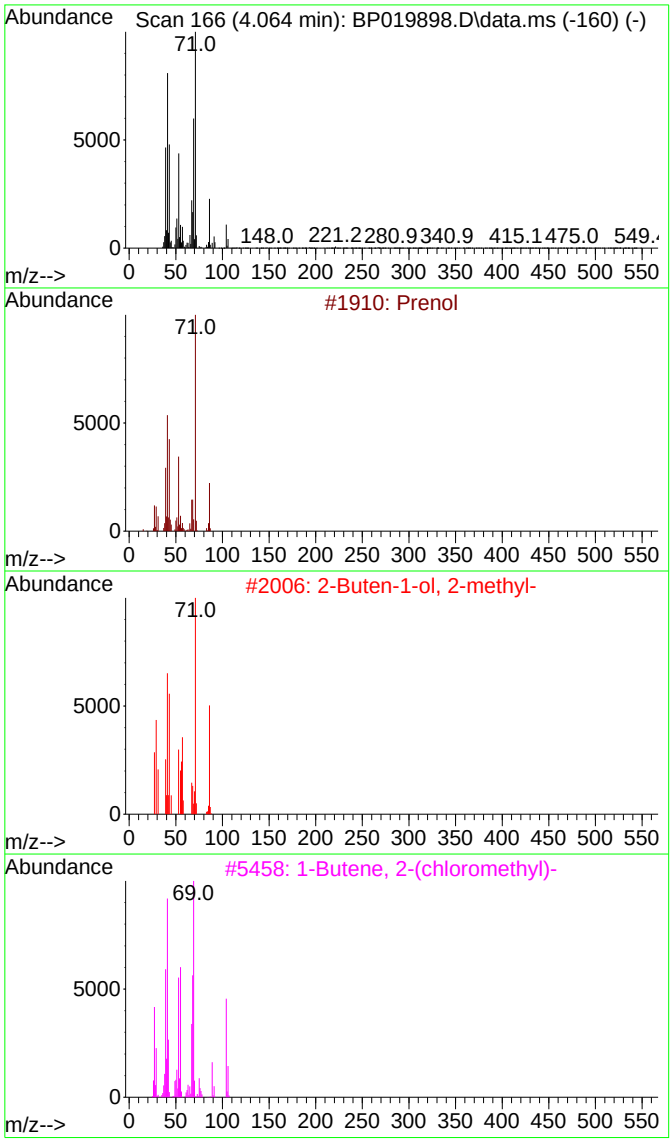
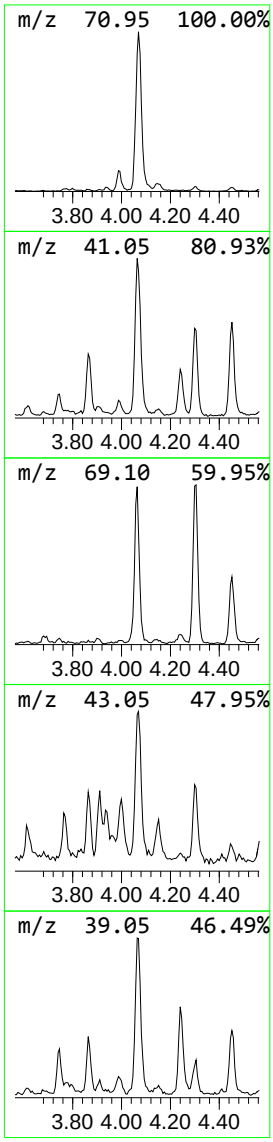
Peak Number 3 Prenol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.064	11.07 ng	318199	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	74
2	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	72
3	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	50
4	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	43
5	1-Butene, 1-chloro-3-methyl-	104	C5H9Cl	023010-00-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

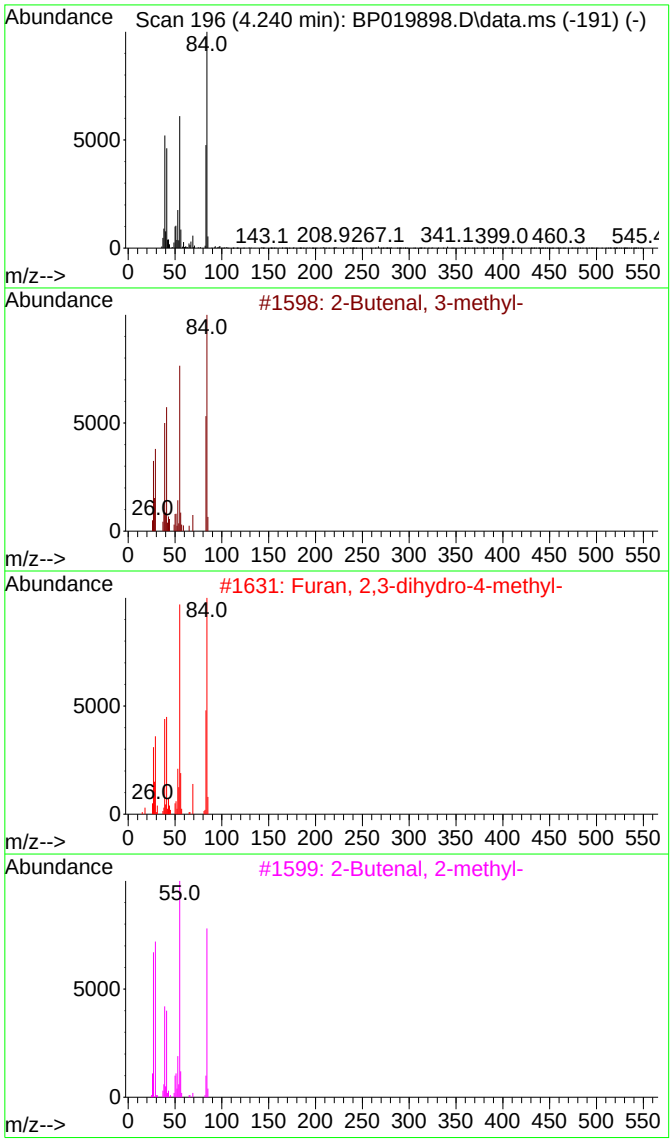
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

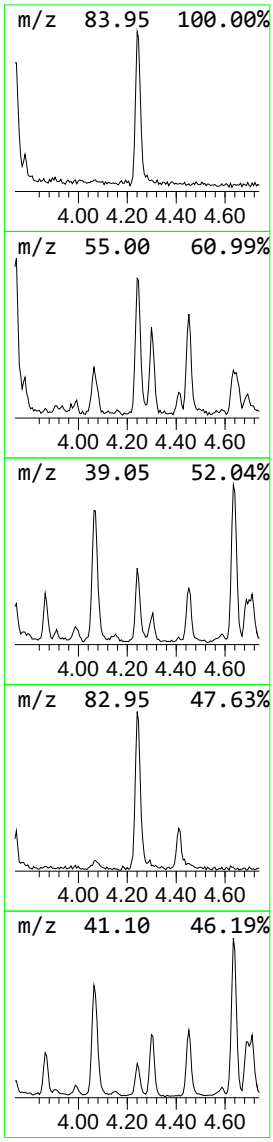
****

Peak Number 4 2-Butenal, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	3.31 ng	95080	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	91
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	72
3	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	64
4	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	50
5	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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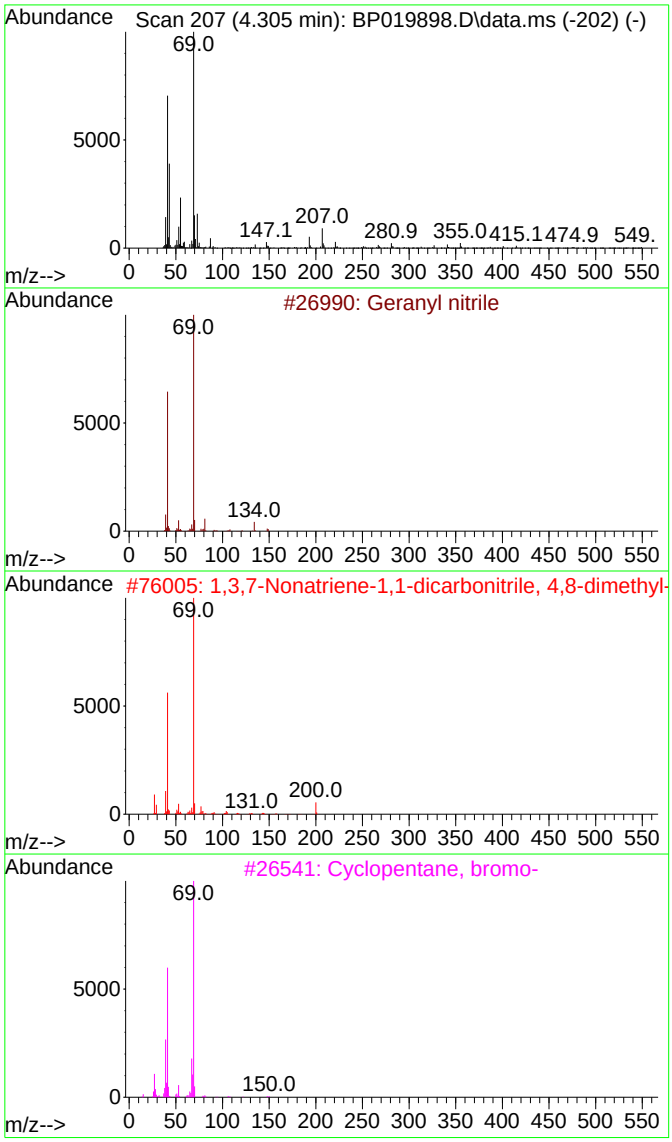
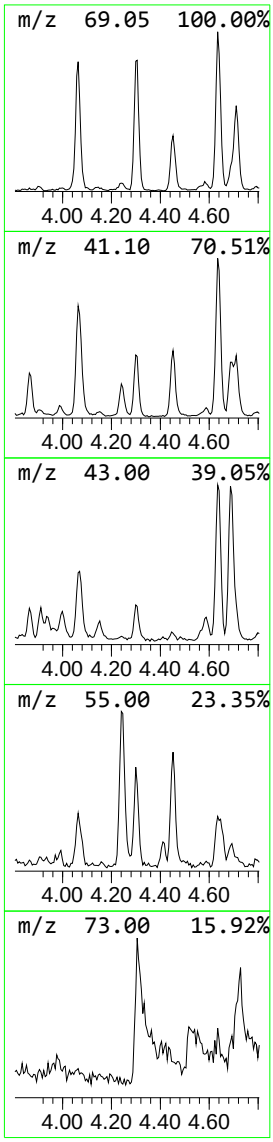
Peak Number 5 Geranyl nitrile Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.305	4.35 ng	125002	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Geranyl nitrile	149	C10H15N	101660-61-1	50
2	1,3,7-Nonatriene-1,1-dicarbonitr...	200	C13H16N2	344401-84-9	50
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	40
4	1,3,7-Nonatriene-1,1-dicarbonitr...	200	C13H16N2	1000162-13-4	40
5	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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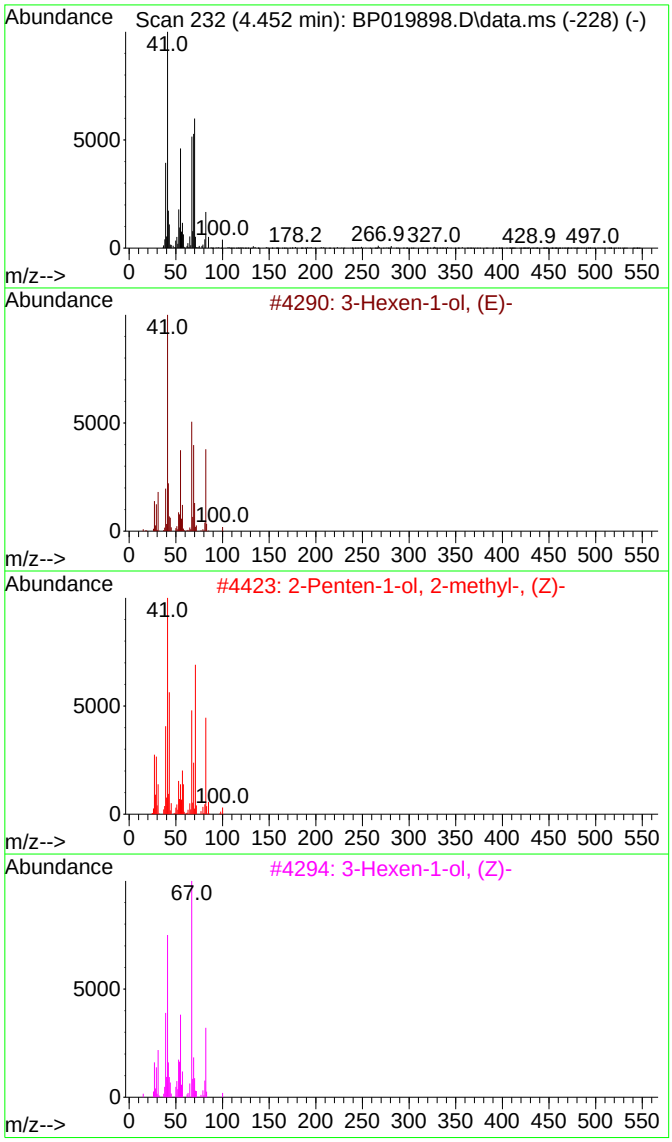
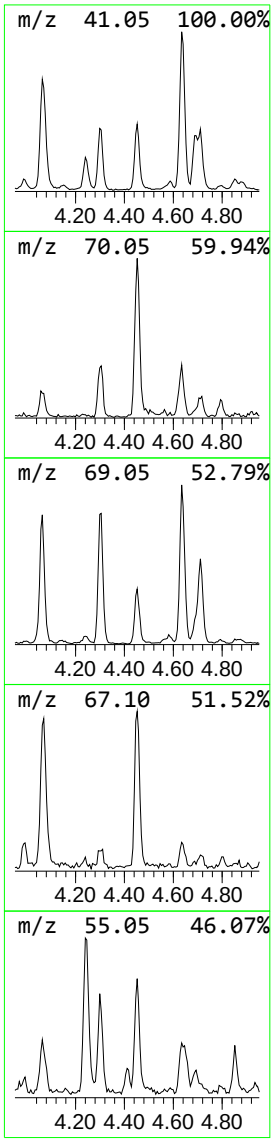
Peak Number 6 unknown4.452 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	3.79 ng	108861	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-1-ol, (E)-	100	C6H12O	000928-97-2	43
2	2-Penten-1-ol, 2-methyl-, (Z)-	100	C6H12O	016958-20-6	38
3	3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	35
4	2,6-Dodecadien-1-al	180	C12H20O	021662-13-5	35
5	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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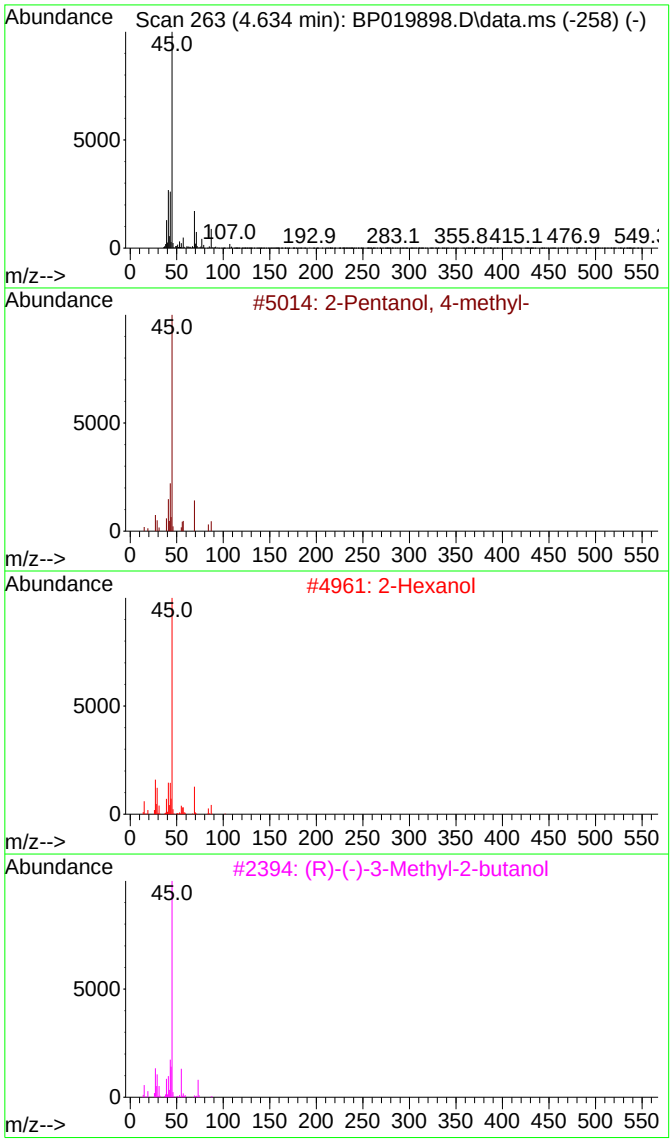
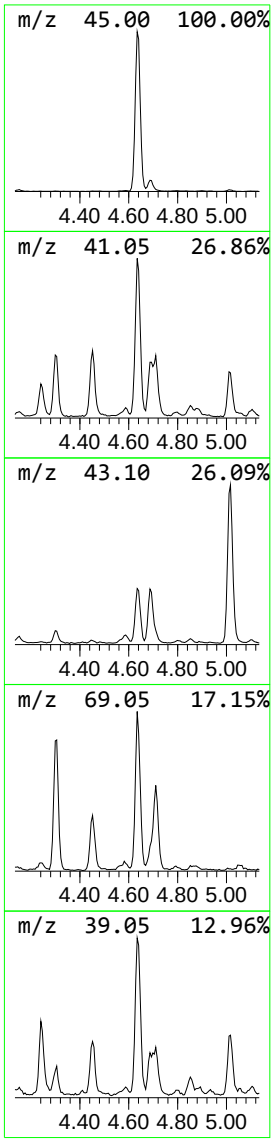
Peak Number 7 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	17.99 ng	517202	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2	2-Hexanol	102	C6H14O	000626-93-7	56
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	53
4	Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	40
5	4-Penten-2-ol	86	C5H10O	000625-31-0	38





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Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

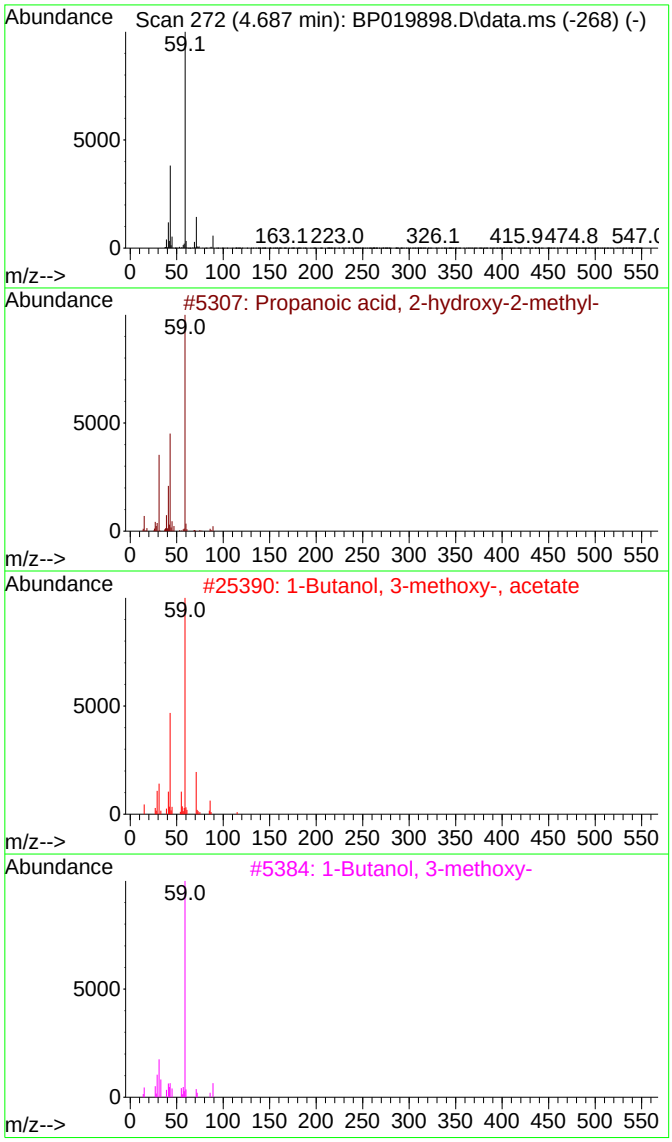
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

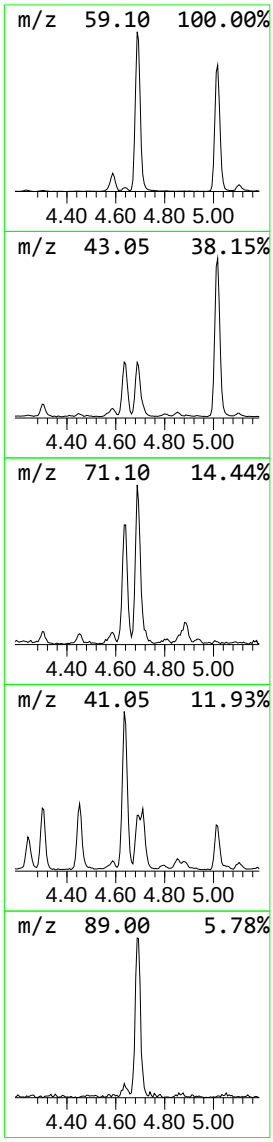
****

Peak Number 8 Propanoic acid, 2-hydroxy-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	12.45 ng	357966	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	64
2	1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	50
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	38
4	Guanidine	59	CH5N3	000113-00-8	9
5	Carbonic acid, 3-pentyl propyl e...	174	C9H18O3	1000325-64-0	9





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Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

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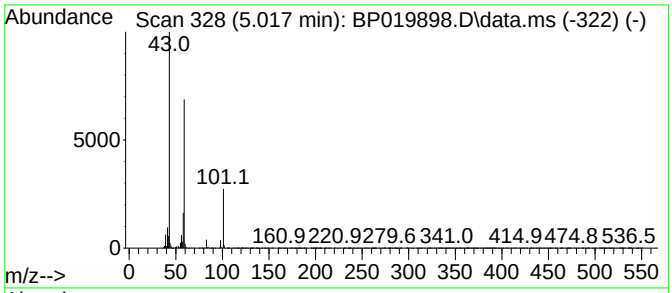
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

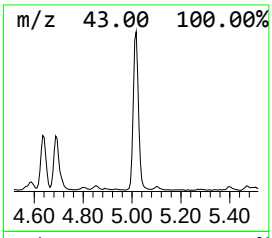
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

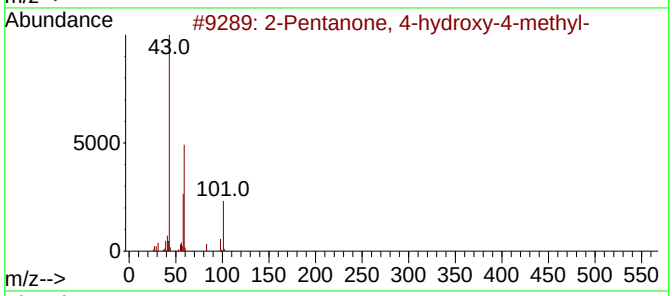
****
Peak Number 9 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

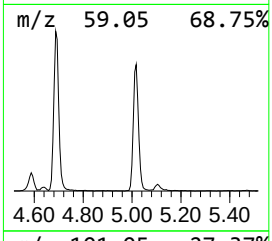
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.017	14.87 ng	427337	1,4-Dichlorobenzene-d4	7.893

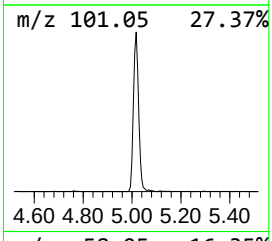
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9

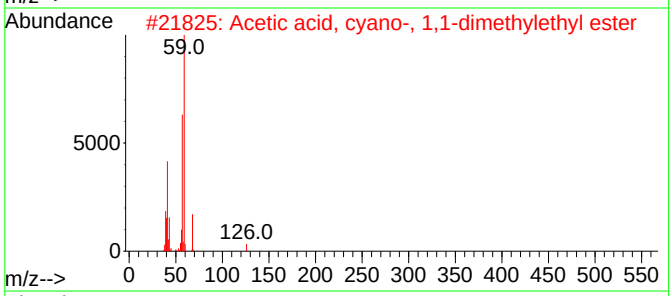


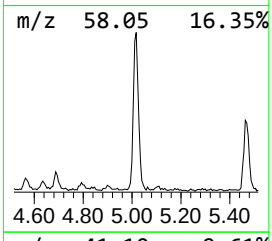


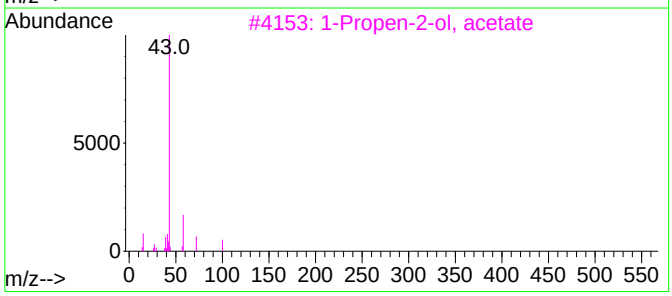


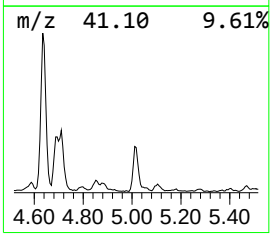












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Acq On : 27 Feb 2024 16:00
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Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

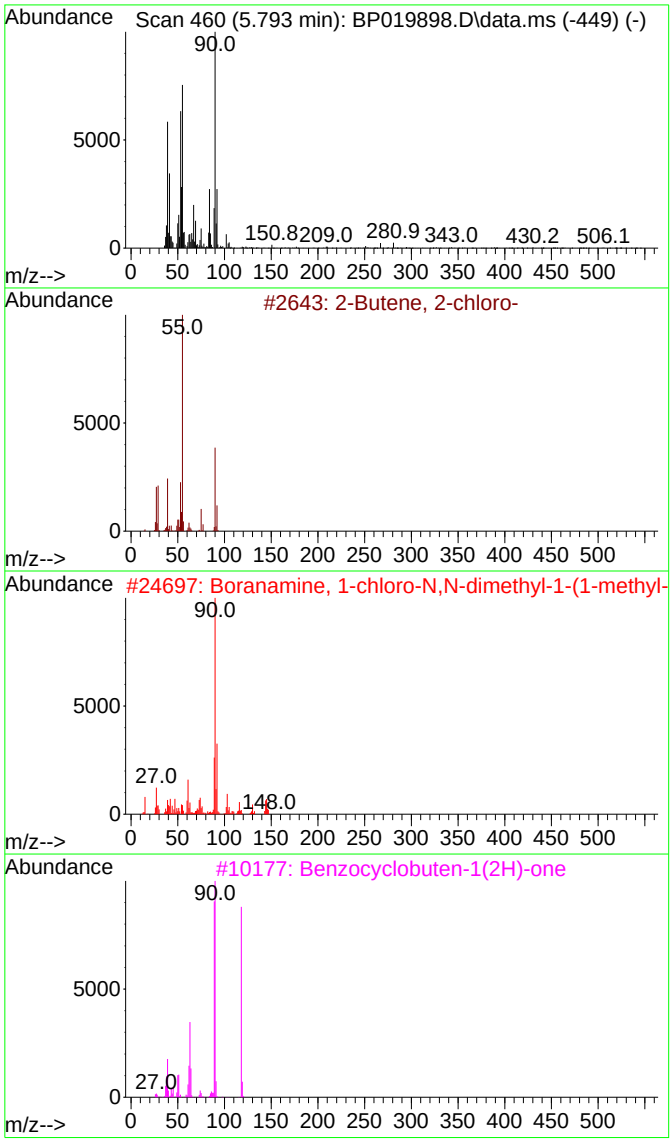
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

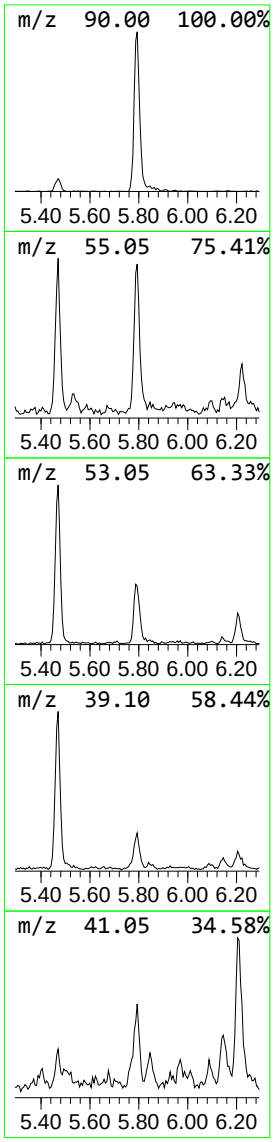
****

Peak Number 10 unknown5.793 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.793	3.26 ng	93672	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-chloro-	90	C4H7Cl	004461-41-0	47
2	Boranamine, 1-chloro-N,N-dimethy...	145	C6H13BClN	051783-28-9	25
3	Benzocyclobuten-1(2H)-one	118	C8H6O	003469-06-5	23
4	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	23
5	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	10





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Sample : P1523-02
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

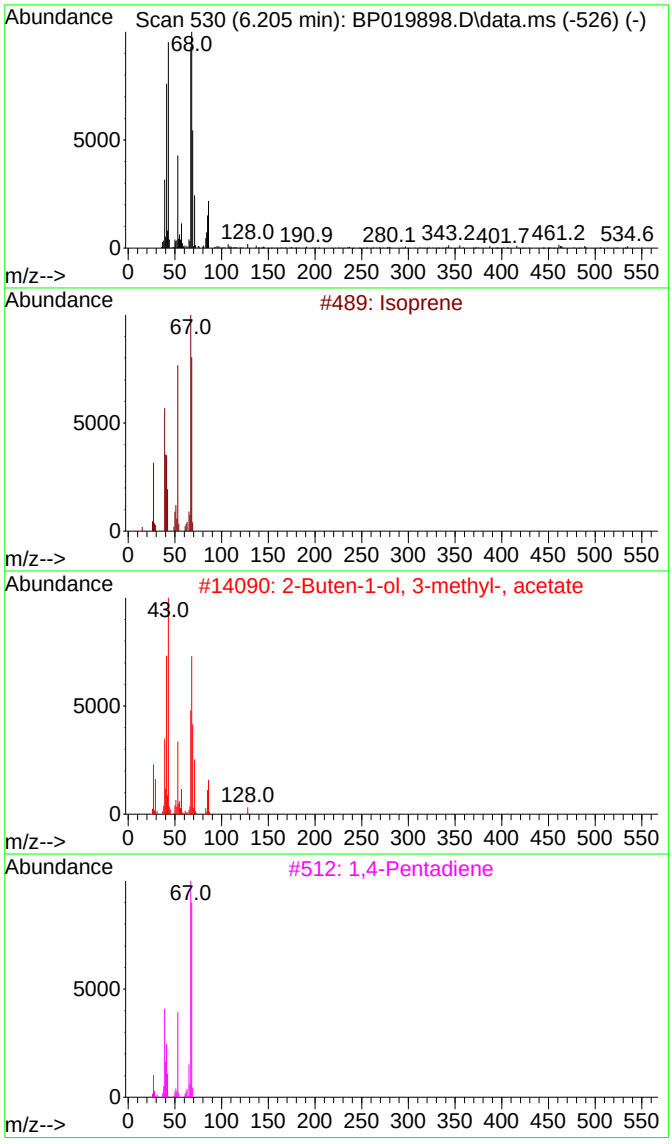
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

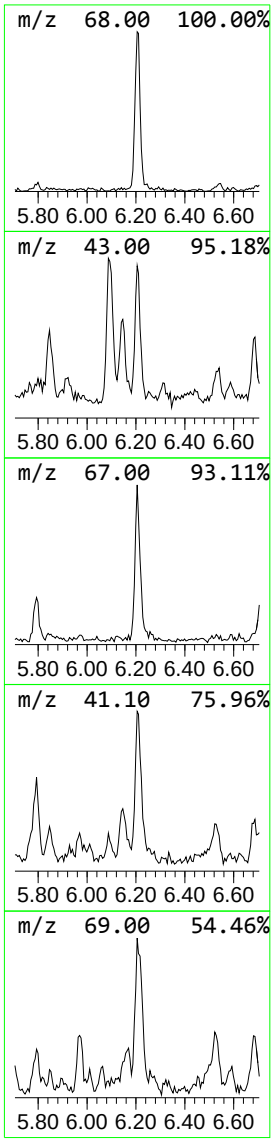
****

Peak Number 11 Isoprene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.205	3.29 ng	94541	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoprene	68	C5H8	000078-79-5	80
2	2-Buten-1-ol, 3-methyl-, acetate	128	C7H12O2	001191-16-8	80
3	1,4-Pentadiene	68	C5H8	000591-93-5	72
4	4-Penten-1-ol, trifluoroacetate	182	C7H9F3O2	1000365-57-8	56
5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	53





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Sample : P1523-02
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

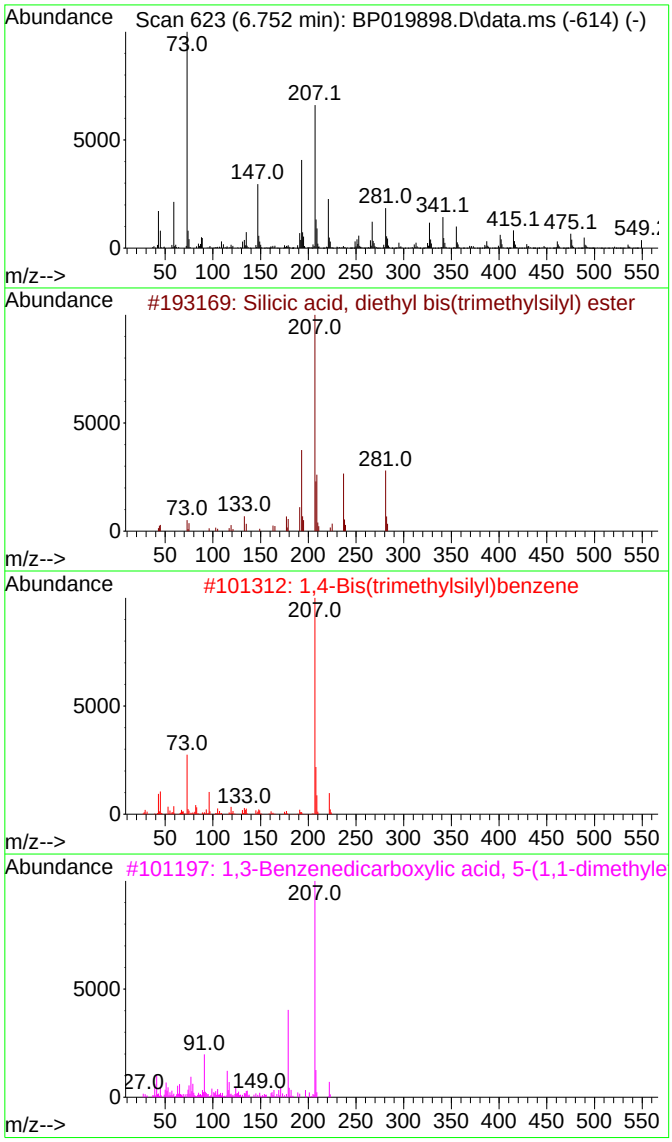
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

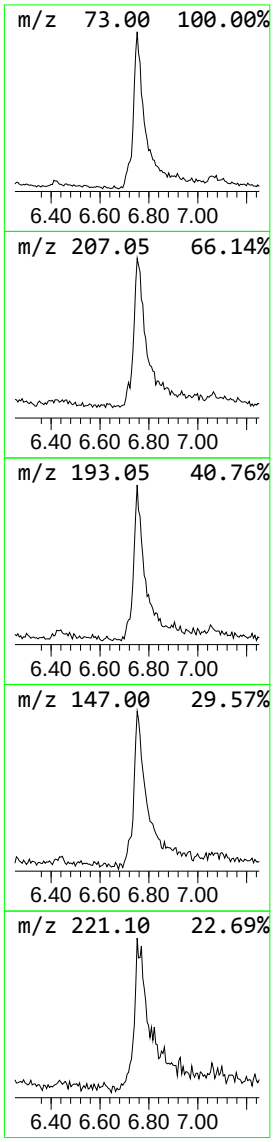
****

Peak Number 12 unknown6.752 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.752	18.80 ng	540455	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silicic acid, diethyl bis(trimet...	296	C10H28O4Si3	003555-45-1	38
2	1,4-Bis(trimethylsilyl)benzene	222	C12H22Si2	013183-70-5	25
3	1,3-Benzenedicarboxylic acid, 5-...	222	C12H14O4	002359-09-3	22
4	2-Methyl-7-phenylindole	207	C15H13N	001140-08-5	22
5	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	22





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Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

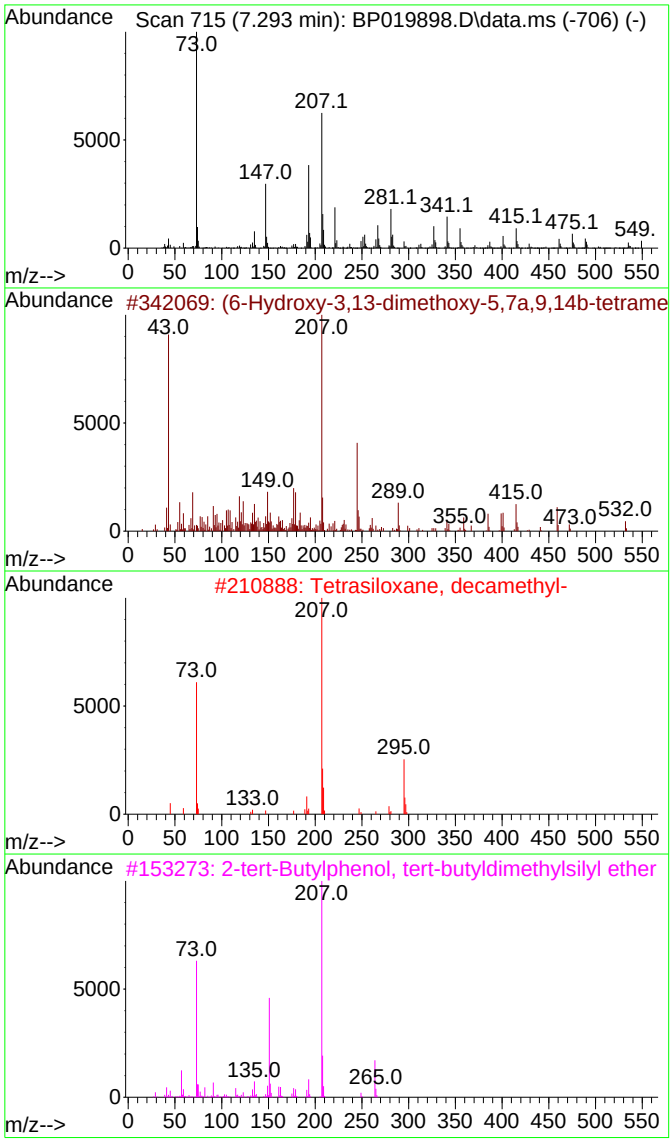
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

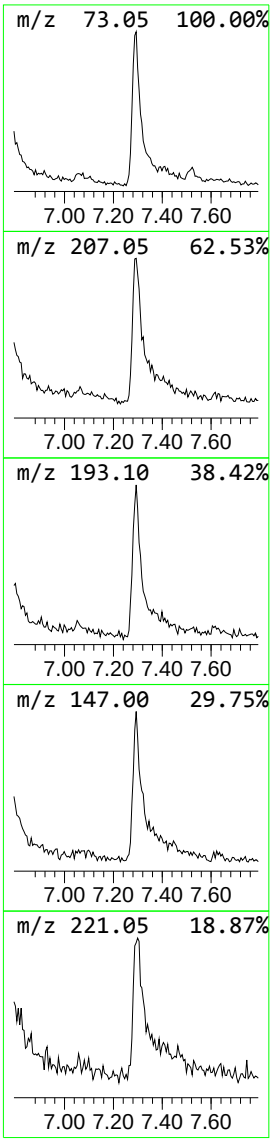
****

Peak Number 13 unknown7.293 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.293	12.76 ng	366707	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6-Hydroxy-3,13-dimethoxy-5,7a,9...	532	C28H36O10	1000496-06-2	25
2	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	22
3	2-tert-Butylphenol, tert-butyldi...	264	C16H28OSi	860465-21-0	22
4	Stannane, tributylethyl-	320	C14H32Sn	019411-60-0	20
5	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	18





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Sample : P1523-02
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ALS Vial : 13 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

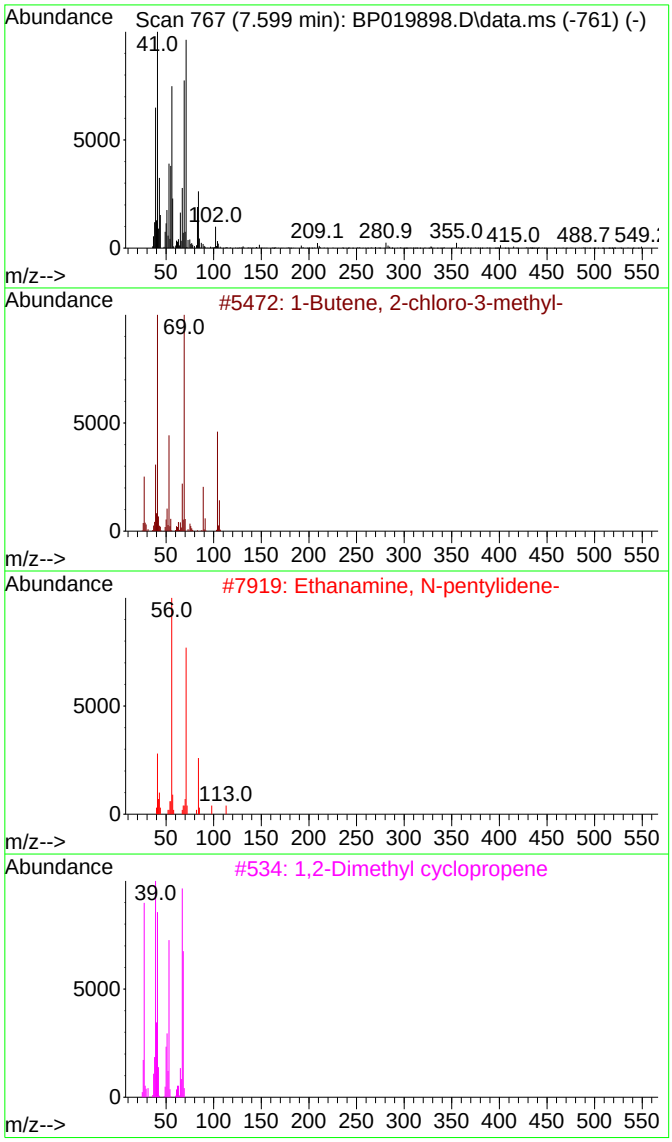
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

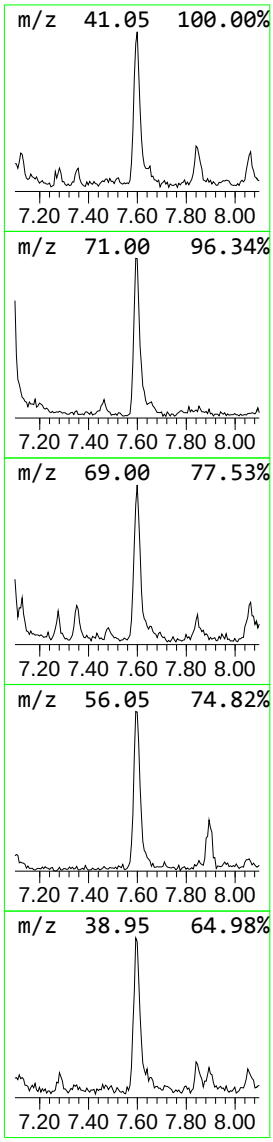
****

Peak Number 14 unknown7.599 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.599	4.51 ng	129730	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	38
2	Ethanamine, N-pentylidene-	113	C7H15N	010599-76-5	27
3	1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	25
4	1-Butene	56	C4H8	000106-98-9	10
5	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	10





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Sample : P1523-02
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Instrument :
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ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

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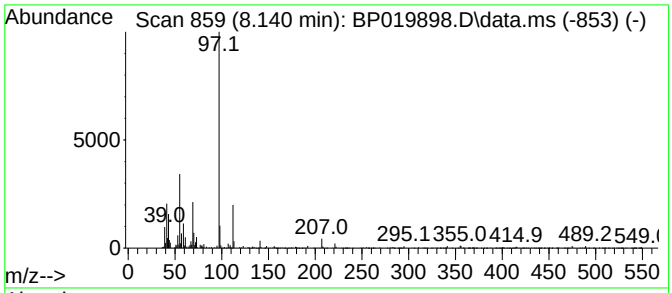
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

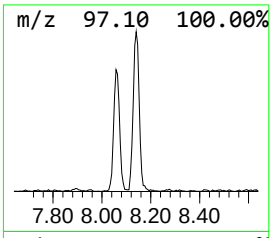
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

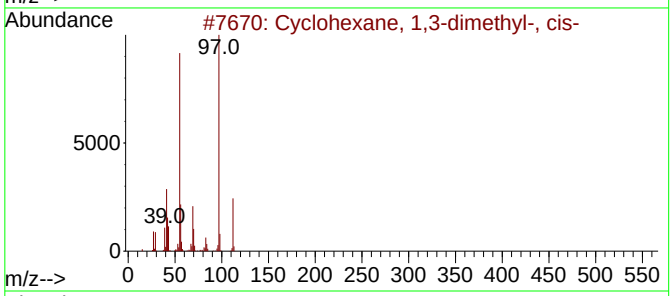
****
Peak Number 15 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 17

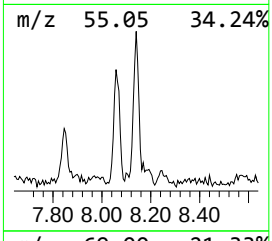
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	3.16 ng	90705	1,4-Dichlorobenzene-d4	7.893

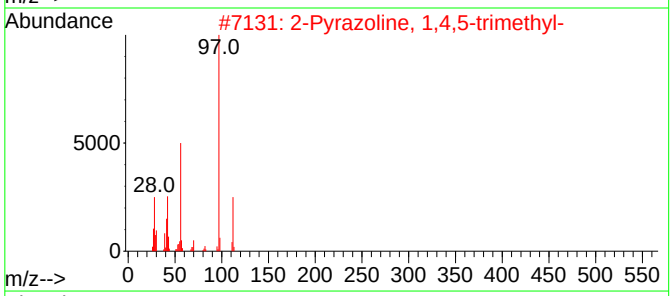
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	64
2	2-Pyrazoline, 1,4,5-trimethyl-	112	C6H12N2	007423-11-2	64
3	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	64
4	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	64
5	2-Pentene, 3,4,4-trimethyl-	112	C8H16	000598-96-9	50

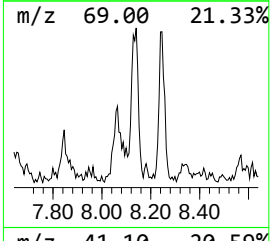


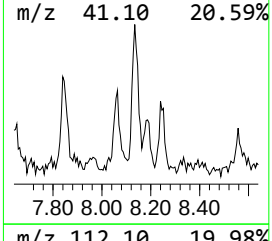


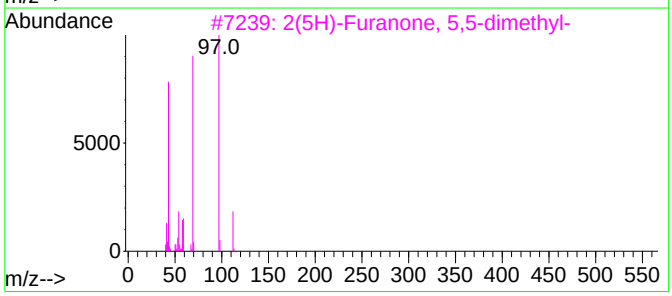


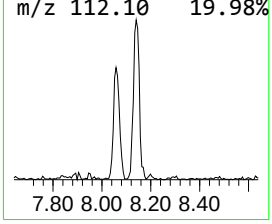












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Sample : P1523-02
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ALS Vial : 13 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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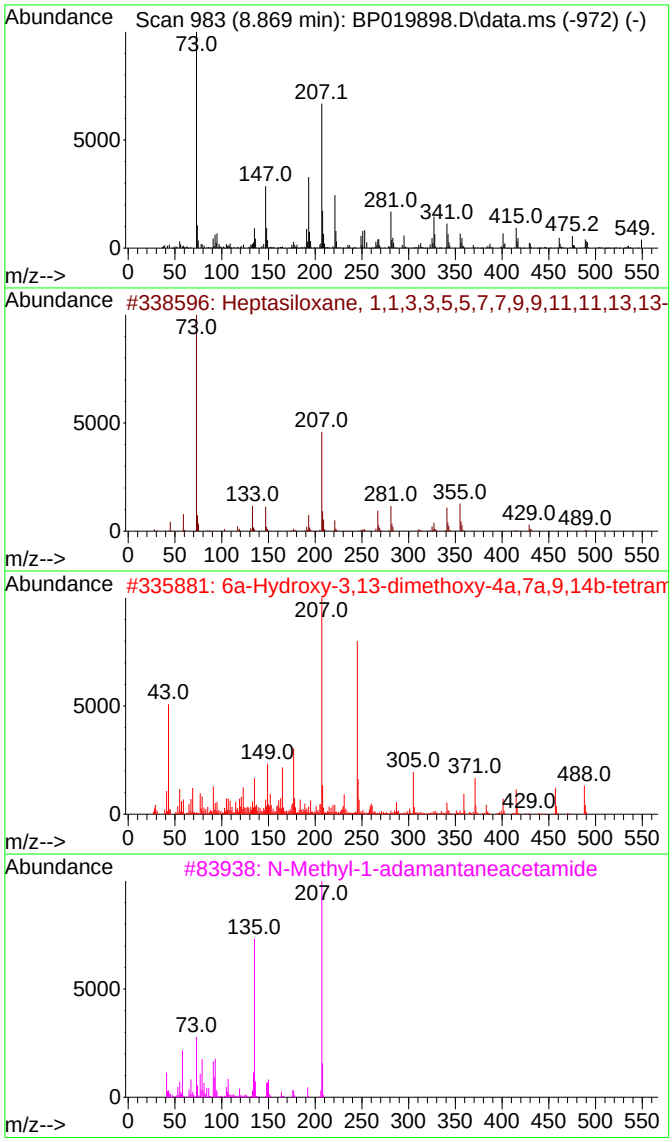
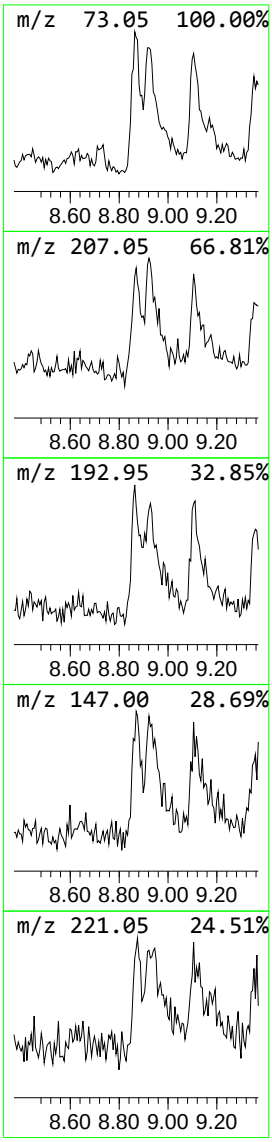
Peak Number 16 unknown8.869 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	2.87 ng	82427	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	46
2	6a-Hydroxy-3,13-dimethoxy-4a,7a,...	488	C26H32O9	1010475-65-9	42
3	N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	30
4	6-Fluoroindole, TMS derivative	207	C11H14FNSi	1000468-35-0	30
5	Stannane, tributylethyl-	320	C14H32Sn	019411-60-0	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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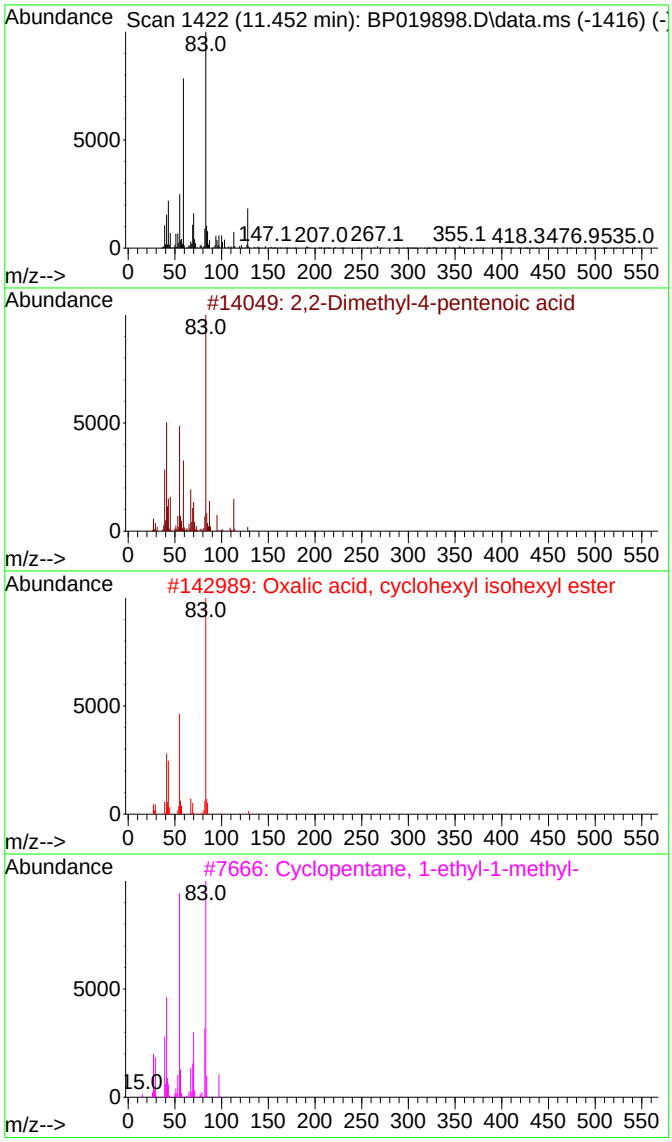
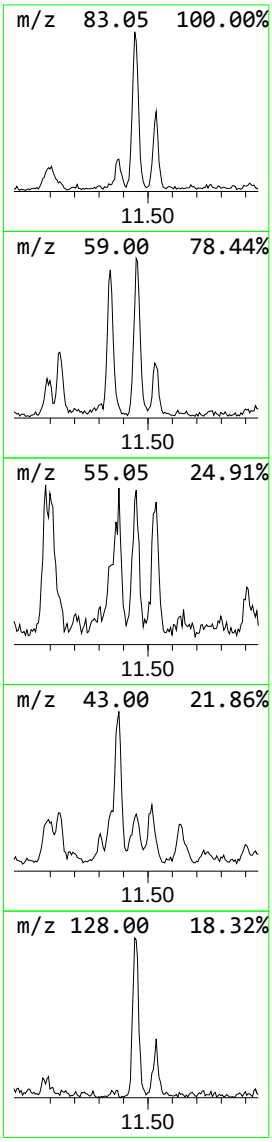
Peak Number 17 unknown11.451 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.451	2.68 ng	111168	Naphthalene-d8	10.699

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	37
2	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	35
3	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	35
4	2-Butenoic acid, 3-methyl-, ethy...	128	C7H12O2	000638-10-8	32
5	Oxalic acid, cyclohexyl hexyl ester	256	C14H24O4	1000309-30-8	25





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Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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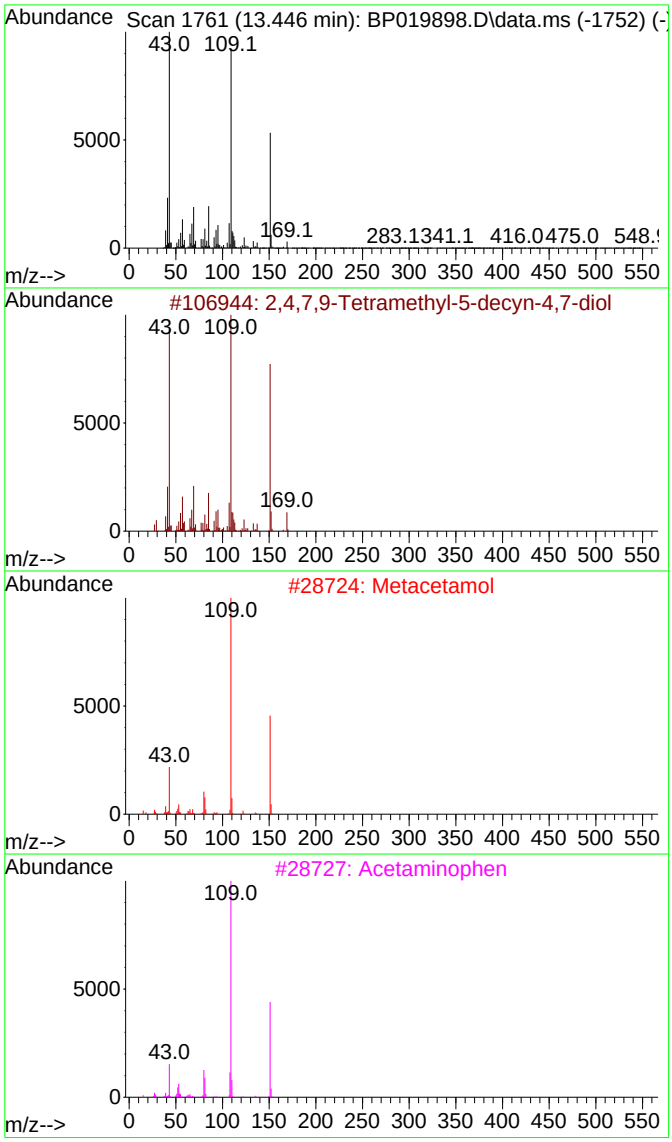
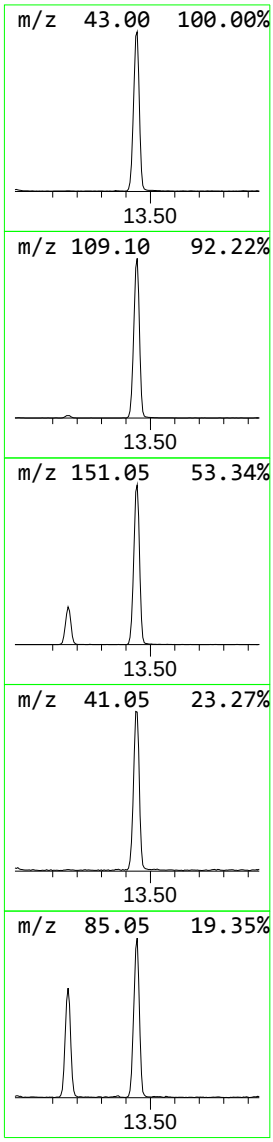
Peak Number 18 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.446	36.69 ng	2126040	Acenaphthene-d10	14.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	50
3	Acetaminophen	151	C8H9NO2	000103-90-2	50
4	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	50
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50





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Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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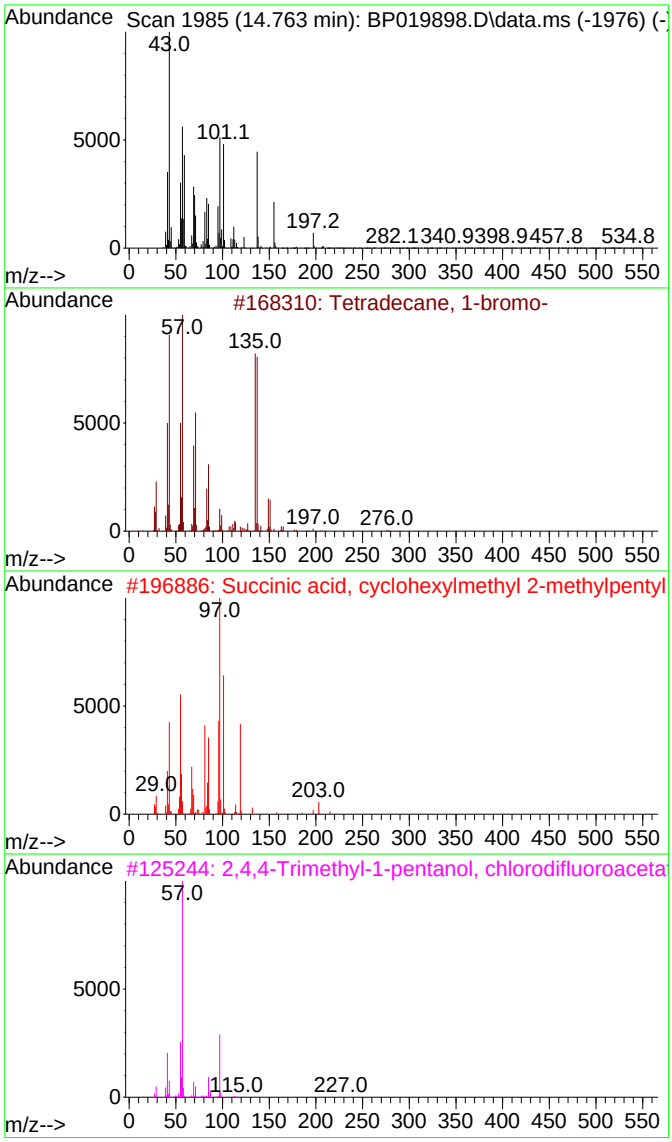
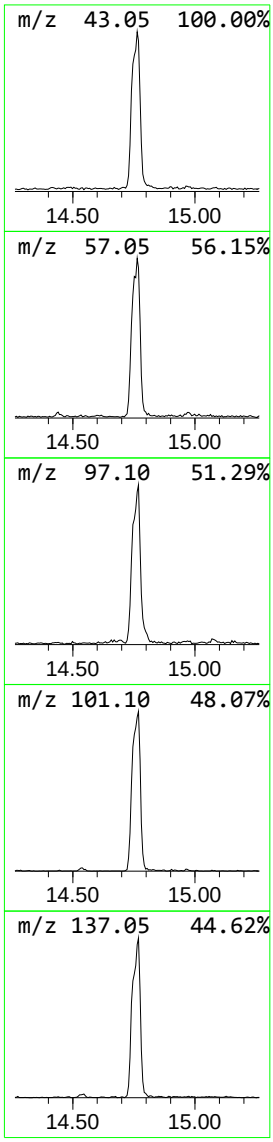
Peak Number 19 unknown14.763 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	11.19 ng	648384	Acenaphthene-d10	14.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
2	Succinic acid, cyclohexylmethyl ...	298	C17H30O4	1000389-65-4	10
3	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
4	2-(Diethylamino)acetonitrile	112	C6H12N2	003010-02-4	10
5	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	053783-91-8	10





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Operator : MA/JU
Sample : P1523-02
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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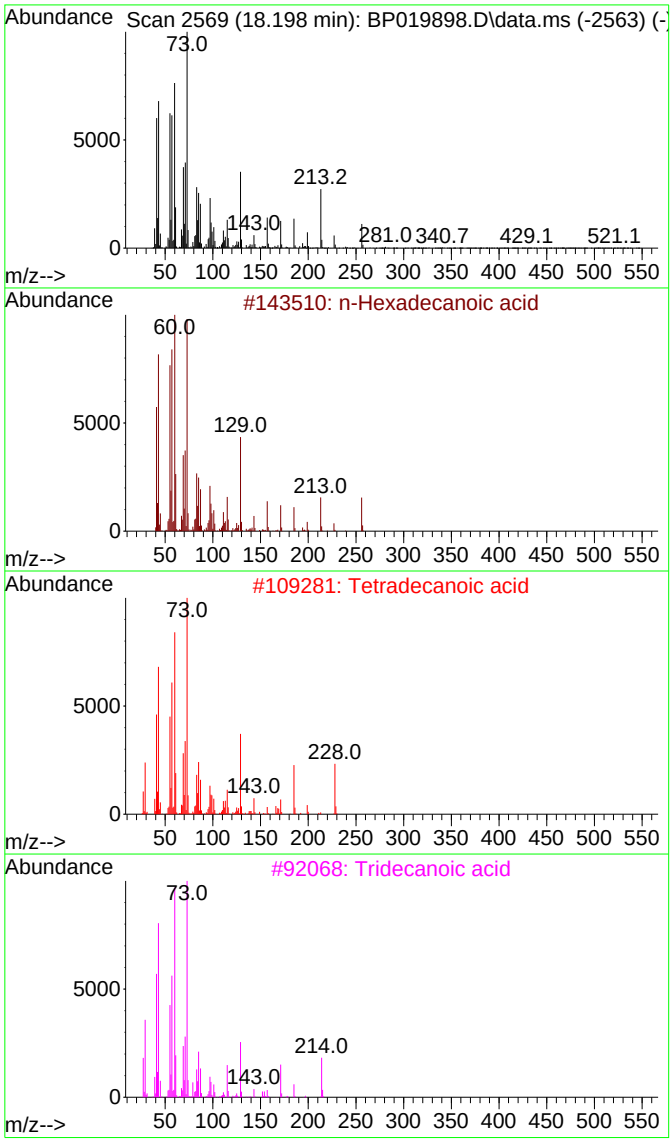
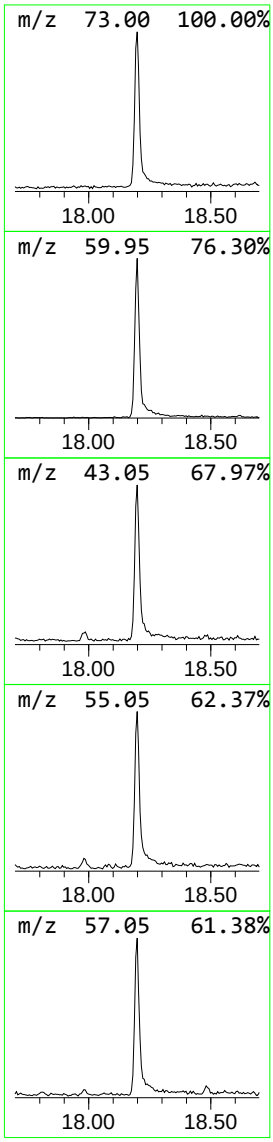
Peak Number 20 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	6.96 ng	512631	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019898.D
Acq On : 27 Feb 2024 16:00
Operator : MA/JU
Sample : P1523-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240764-COMPOSITE-39N-N-3-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-ol	3.123	104.9	ng	3016100	1	7.893	574869	20.0
2-Butenal, 2-me...	3.746	3.0	ng	87516	1	7.893	574869	20.0
Prenol	4.064	11.1	ng	318199	1	7.893	574869	20.0
2-Butenal, 3-me...	4.240	3.3	ng	95080	1	7.893	574869	20.0
Geranyl nitrile	4.305	4.3	ng	125002	1	7.893	574869	20.0
unknown4.452	4.452	3.8	ng	108861	1	7.893	574869	20.0
2-Pentanol, 4-m...	4.634	18.0	ng	517202	1	7.893	574869	20.0
Propanoic acid,...	4.687	12.4	ng	357966	1	7.893	574869	20.0
2-Pentanone, 4-...	5.017	14.9	ng	427337	1	7.893	574869	20.0
unknown5.793	5.793	3.3	ng	93672	1	7.893	574869	20.0
Isoprene	6.205	3.3	ng	94541	1	7.893	574869	20.0
unknown6.752	6.752	18.8	ng	540455	1	7.893	574869	20.0
unknown7.293	7.293	12.8	ng	366707	1	7.893	574869	20.0
unknown7.599	7.599	4.5	ng	129730	1	7.893	574869	20.0
Cyclohexane, 1,...	8.140	3.2	ng	90705	1	7.893	574869	20.0
unknown8.869	8.869	2.9	ng	82427	1	7.893	574869	20.0
unknown11.451	11.451	2.7	ng	111168	2	10.699	828630	20.0
2,4,7,9-Tetrame...	13.446	36.7	ng	2126040	3	14.540	1158840	20.0
unknown14.763	14.763	11.2	ng	648384	3	14.540	1158840	20.0
n-Hexadecanoic ...	18.198	7.0	ng	512631	4	17.298	1473420	20.0