LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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: BP019915.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	17	rVB	2680300	2923866	73.76%	9.450%
2	3.740	107	111	119	rBV2	42774	77517	1.96%	0.251%
3	3.864	127	132	136	rBV	49843	64933	1.64%	0.210%
4	4.064	159	166	174	rBV2	179657	289015	7.29%	0.934%
5	4.234	188	195	201	rBV	54935	85904	2.17%	0.278%
6	4.446	227	231	241	rVB	70138	98755	2.49%	0.319%
7	4.581	248	254	258	rBV2	33007	51901	1.31%	0.168%
8	4.634	258	263	267	rVV	265254	394490	9.95%	1.275%
9	4.687	267	272	281	rVB	162313	244667	6.17%	0.791%
10	5.011	320	327	337	rBV	1064105	1518002	38.29%	4.906%
11	5.464	397	404	412	rBV	694691	1070939	27.02%	3.461%
12	5.787	454	459	464	rBV	35253	56254	1.42%	0.182%
13	6.087	500	510	515	rBV2	22532	56538	1.43%	0.183%
14	6.199	525	529	537	rVB4	28056	54317	1.37%	0.176%
15	7.064	668	676	682	rBV	914434	1454357	36.69%	4.700%
16	7.587	760	765	775	rBV2	68246	126513	3.19%	0.409%
17	7.887	810	816	823	rVB	385068	597653	15.08%	1.932%
18	8.052	837	844	850	rBV2	28907	52119	1.31%	0.168%
19	8.128	851	857	862	rBV3	41919	75231	1.90%	0.243%
20	8.858	976	981	987	rBV3	31244	73593	1.86%	0.238%
21	9.063	1008	1016	1027	rBV	800135	1394902	35.19%	4.508%
22	9.352	1057	1065	1069	rBV8	18776	48643	1.23%	0.157%
23	9.422	1069	1077	1087	rVV	1261450	2357495	59.47%	7.619%
24	10.052	1179	1184	1189	rBV5	23786	53416	1.35%	0.173%
25	10.557	1262	1270	1275	rBV2	26291	49837	1.26%	0.161%
26	10.687	1285	1292	1309	rVB	436795	793302	20.01%	2.564%
27	10.887	1319	1326	1334	rBV3	22525	50936	1.28%	0.165%
28	11.075	1349	1358	1364	rBV5	43676	131954	3.33%	0.426%
29	11.134	1364	1368	1374	rVB3	25674	49598	1.25%	0.160%
30	11.340	1398	1403	1405	rBV2	26798	41081	1.04%	0.133%
31	11.369	1406	1408	1413	rVB2	31566	42310	1.07%	0.137%
32	11.446	1414	1421	1427	rVV2	43701	80932	2.04%	0.262%
33	11.516	1428	1433	1440	rVB4	23628	45187	1.14%	0.146%
34	13.157	1705	1712	1723	rBV	2070177	3001534	75.72%	9.701%
35	13.298	1729	1736	1743	rBV	188201	320489	8.08%	1.036%
36	13.587	1779	1785	1793	rVB	84605	139643	3.52%	0.451%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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	14.457	1927	1933	1940	rBV	80128	168071	4.24%	0.543%
38	14.534	1940	1946	1954	rVB	665282	994721	25.09%	3.215%
39	15.140	2039	2049	2063	rBV3	55151	209561	5.29%	0.677%
40	15.369	2084	2088	2094	rBV	28637	43081	1.09%	0.139%
41	15.934	2176	2184	2193	rBV3	132634	272916	6.88%	0.882%
42	16.028	2195	2200	2208	rVB	612369	934532	23.57%	3.020%
43	16.269	2235	2241	2248	rBV	270395	433547	10.94%	1.401%
44	17.069	2371	2377	2382	rBV	363801	581474	14.67%	1.879%
45	17.110	2382	2384	2391	rVB	40359	57162	1.44%	0.185%
46	17.292	2409	2415	2421	rBV	711998	1080944	27.27%	3.493%
47	18.192	2563	2568	2577	rBV	248738	423925	10.69%	1.370%
48	18.269	2577	2581	2591	rVB	98391	165673	4.18%	0.535%
49	19.316	2755	2759	2766	rBV	49712	69744	1.76%	0.225%
50	19.433	2775	2779	2791	rBV2	137957	239539	6.04%	0.774%
51	19.663	2815	2818	2821	rBV	38124	44790	1.13%	0.145%
52	19.869	2847	2853	2861	rBV	3221396	3964093	100.00%	12.812%
53	20.875	3022	3024	3030	rVB	41943	48322	1.22%	0.156%
54	21.122	3062	3066	3072	rBV	235046	299978	7.57%	0.969%
55	21.322	3097	3100	3104	rVB	85579	104376	2.63%	0.337%
56	21.398	3108	3113	3118	rBV	970293	1301650	32.84%	4.207%
57	23.821	3518	3525	3535	rVB	732112	1535680	38.74%	4.963%

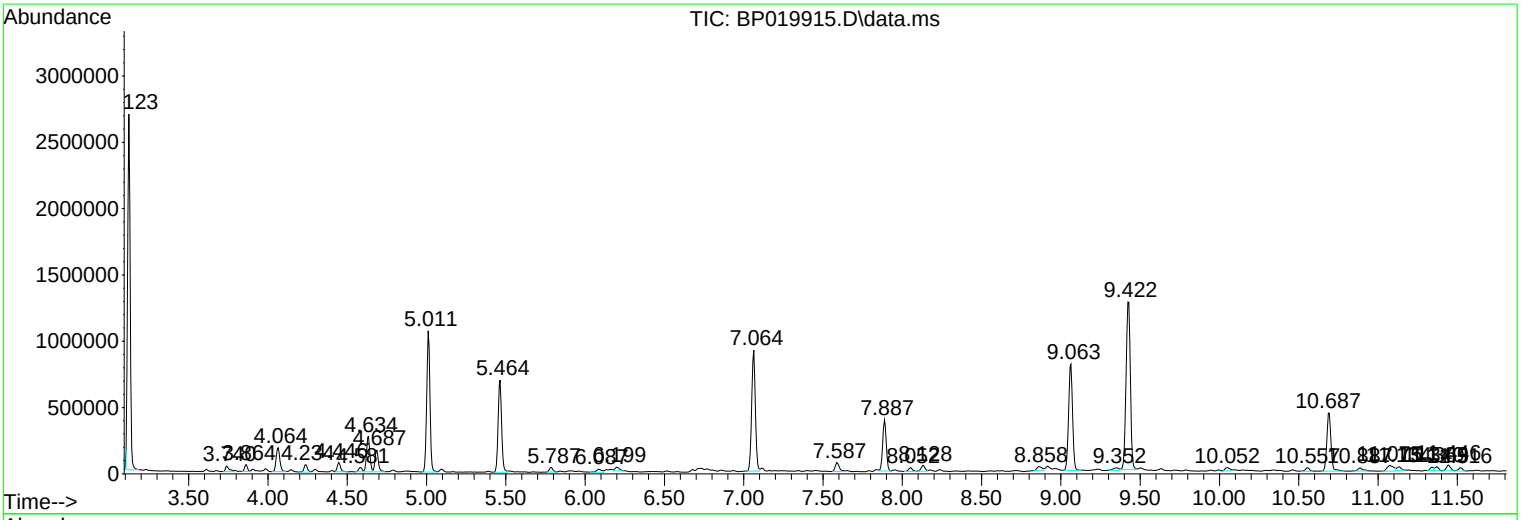
Sum of corrected areas: 30941602

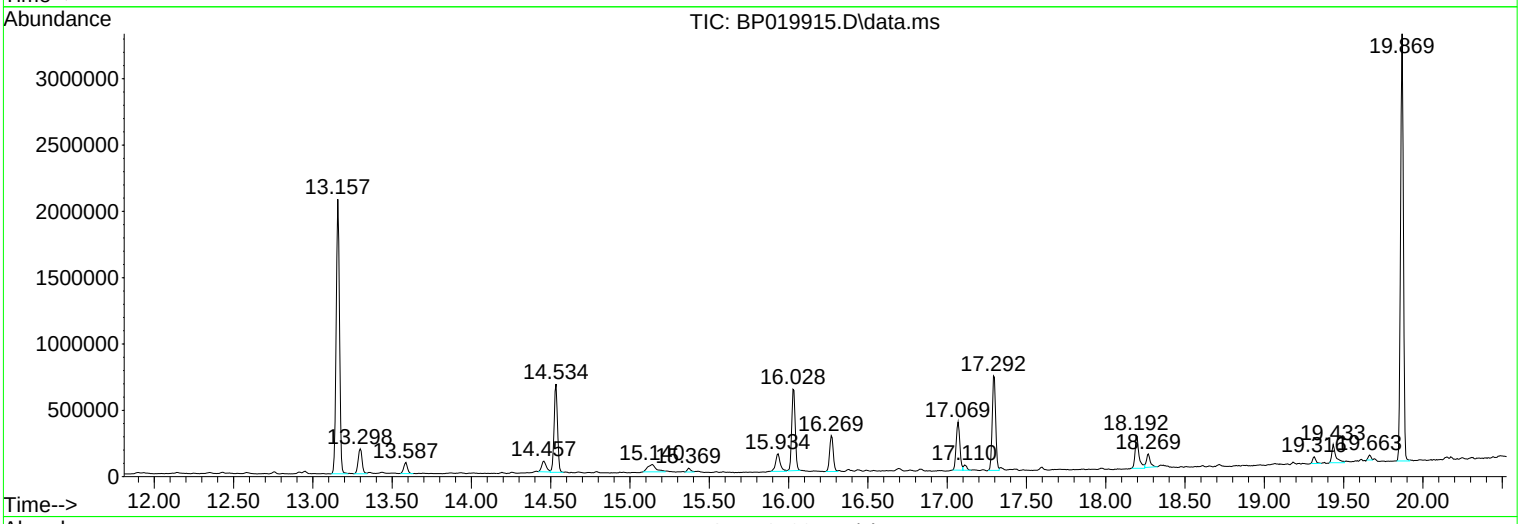
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

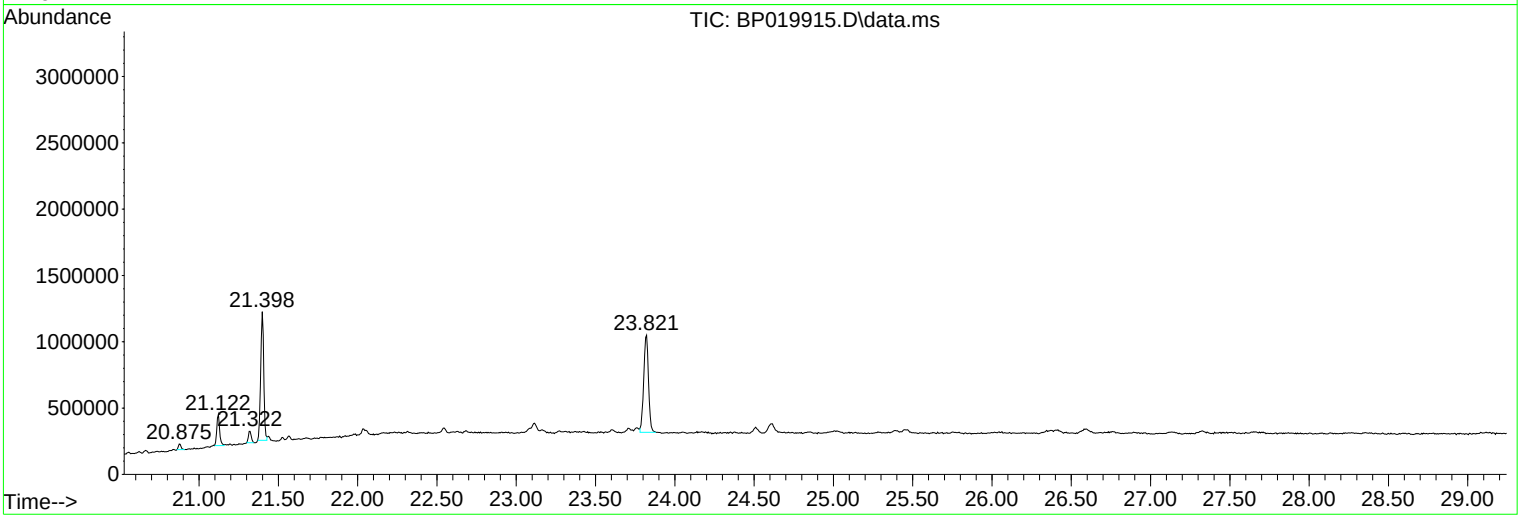
Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

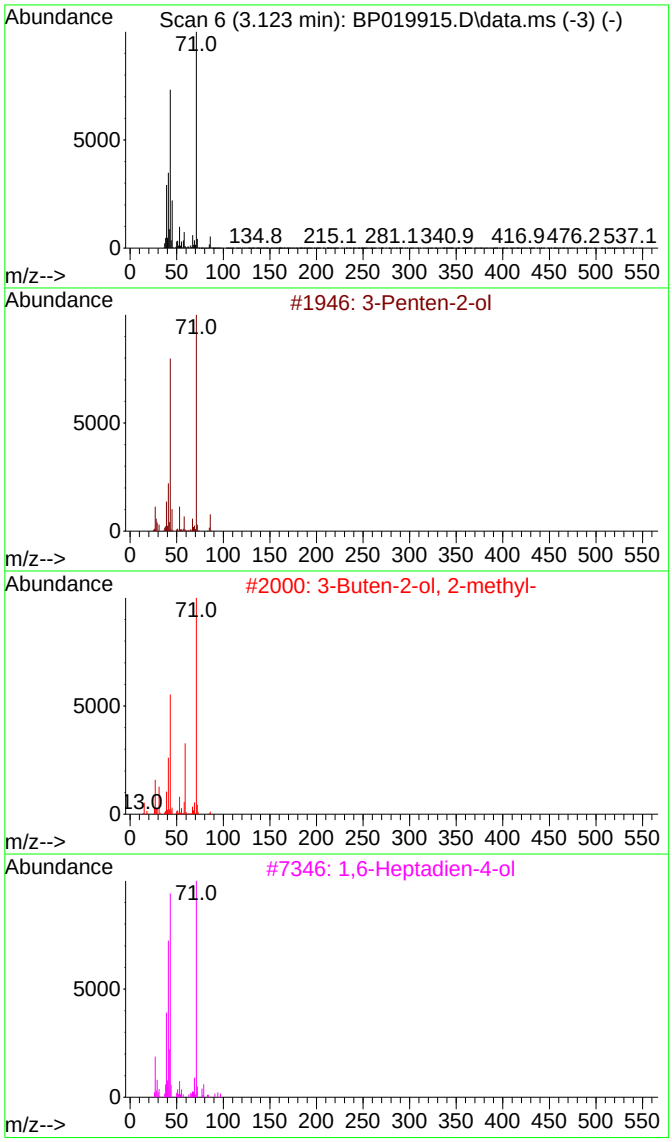
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

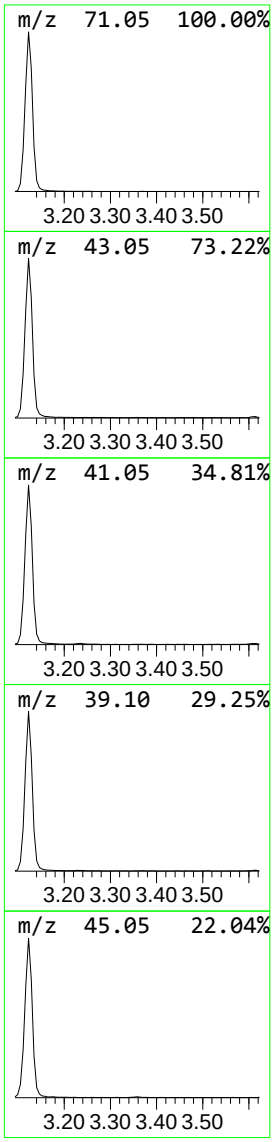
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.123	97.84 ng	2923870	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	87
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
3	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	53
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50
5	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

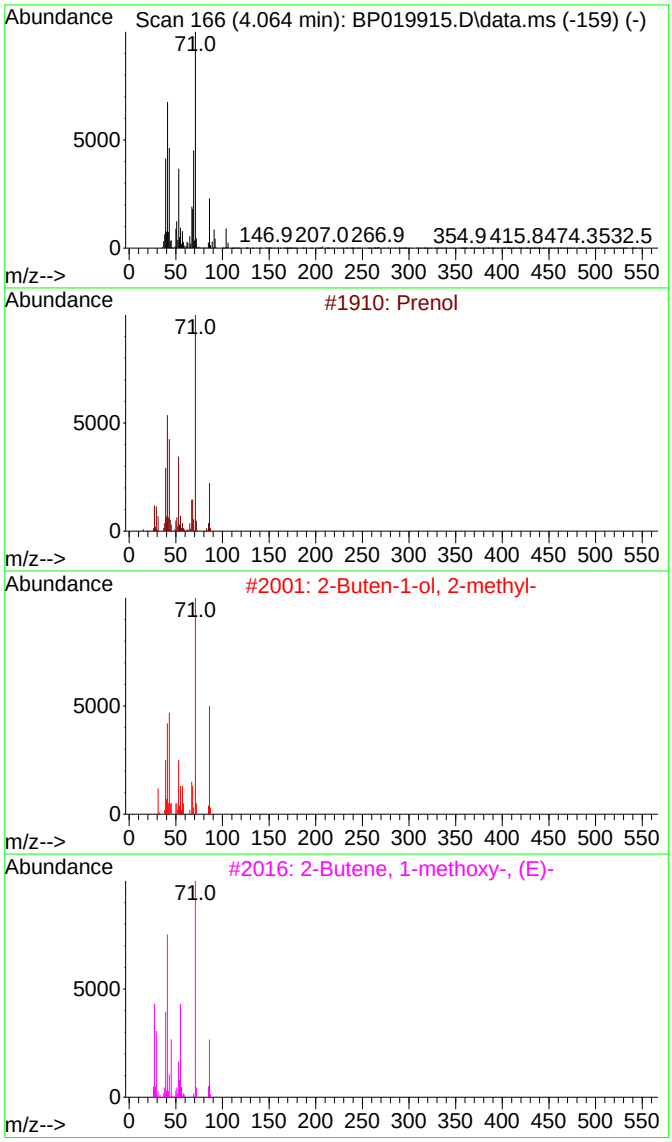
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

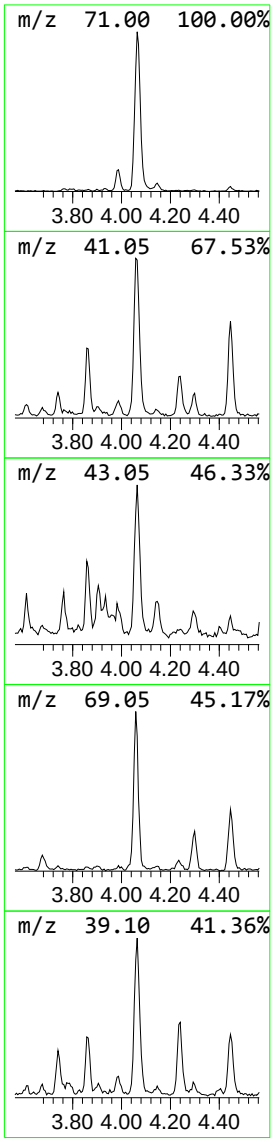
****

Peak Number 2 Prenol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.064	9.67 ng	289015	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	70
2	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	62
3	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	53
4	3-Penten-2-ol	86	C5H10O	001569-50-2	50
5	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

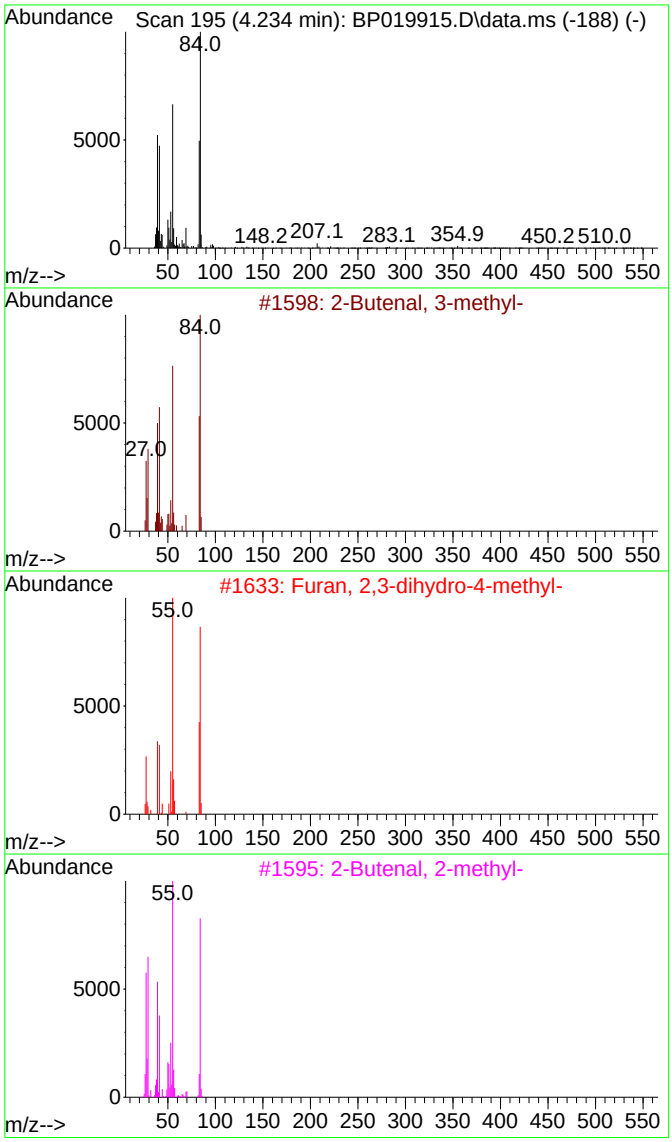
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

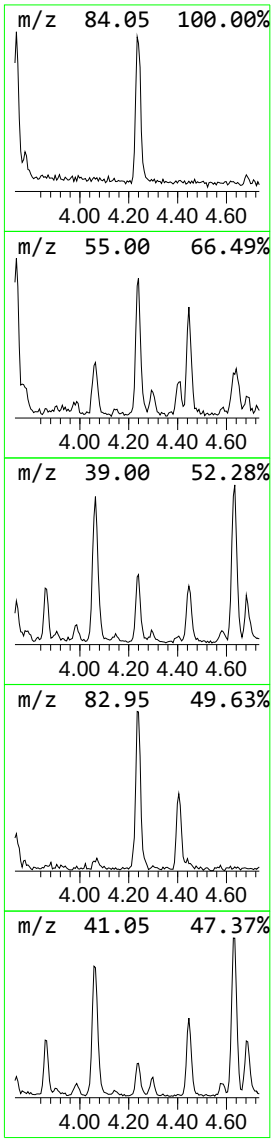
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butenal, 3-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.234	2.87 ng	85904	1,4-Dichlorobenzene-d4	7.887

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	59
3	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	47
4	2-Pentenal, (E)-	84	C5H8O	001576-87-0	47
5	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

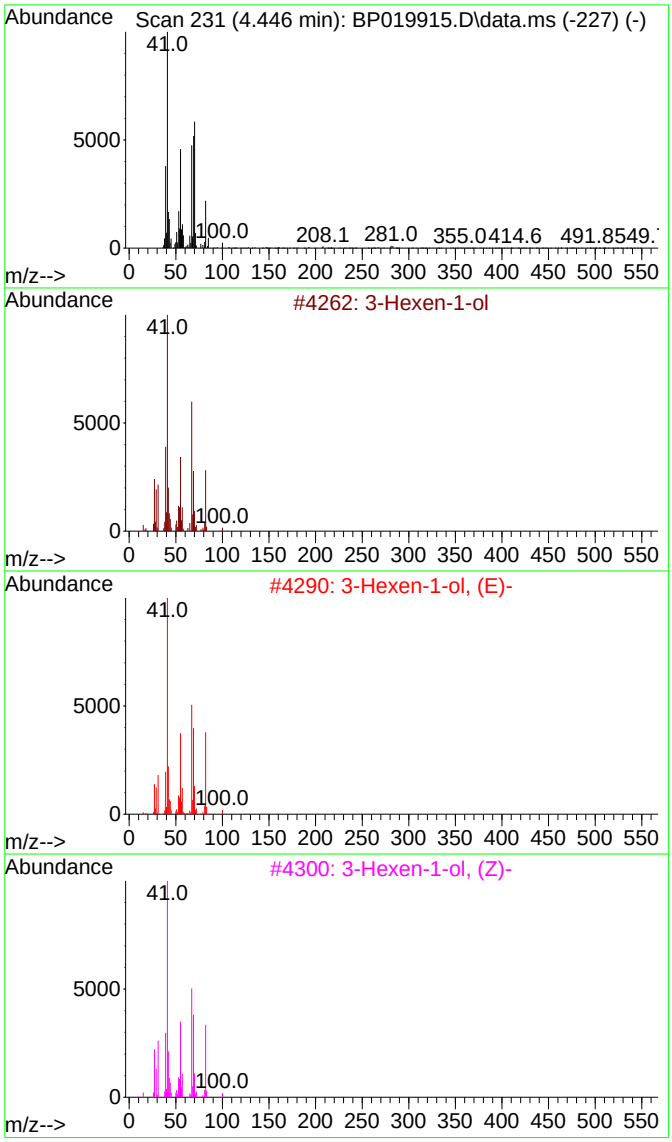
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

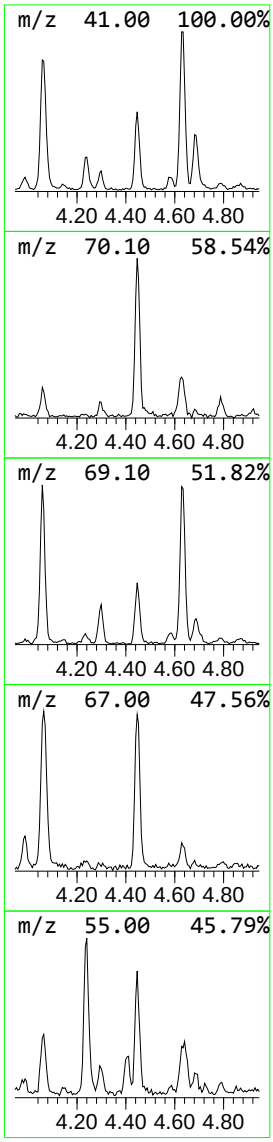
****

Peak Number 4 3-Hexen-1-ol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	3.30 ng	98755	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-1-ol	100	C6H12O	000544-12-7	50
2	3-Hexen-1-ol, (E)-	100	C6H12O	000928-97-2	47
3	3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	43
4	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	38
5	2,6-Dodecadien-1-al	180	C12H20O	021662-13-5	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

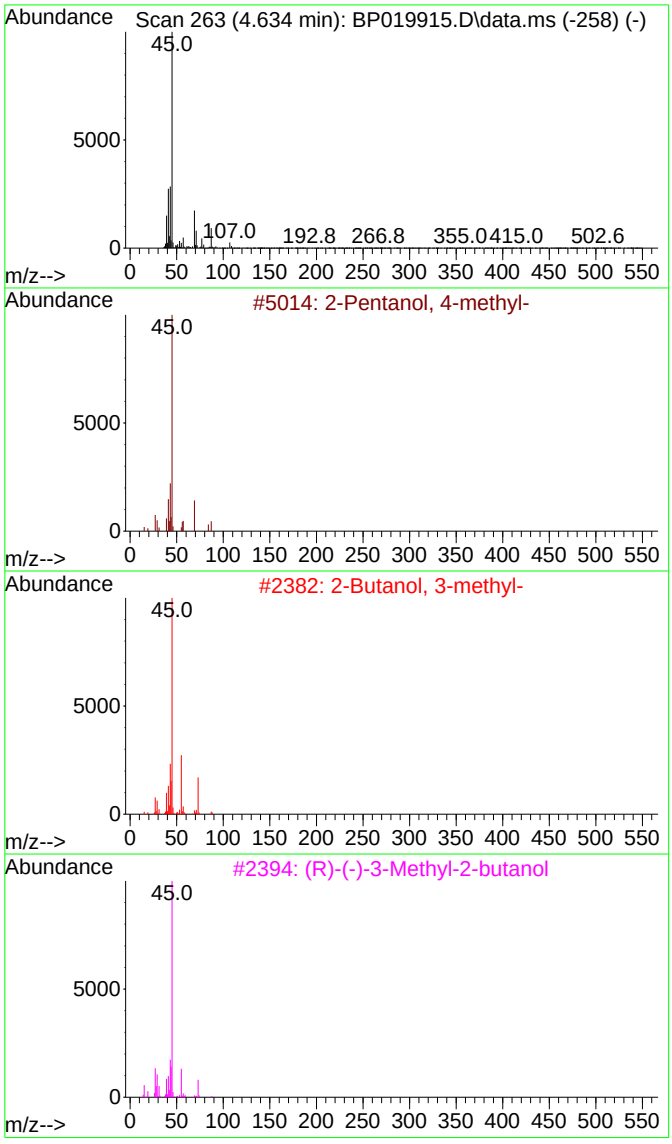
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

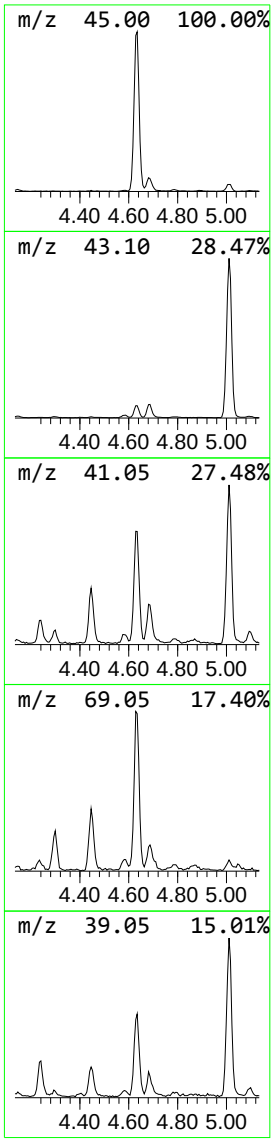
****

Peak Number 5 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.634	13.20 ng	394490	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	53
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	50
4	2-Hexanol	102	C6H14O	000626-93-7	40
5	Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

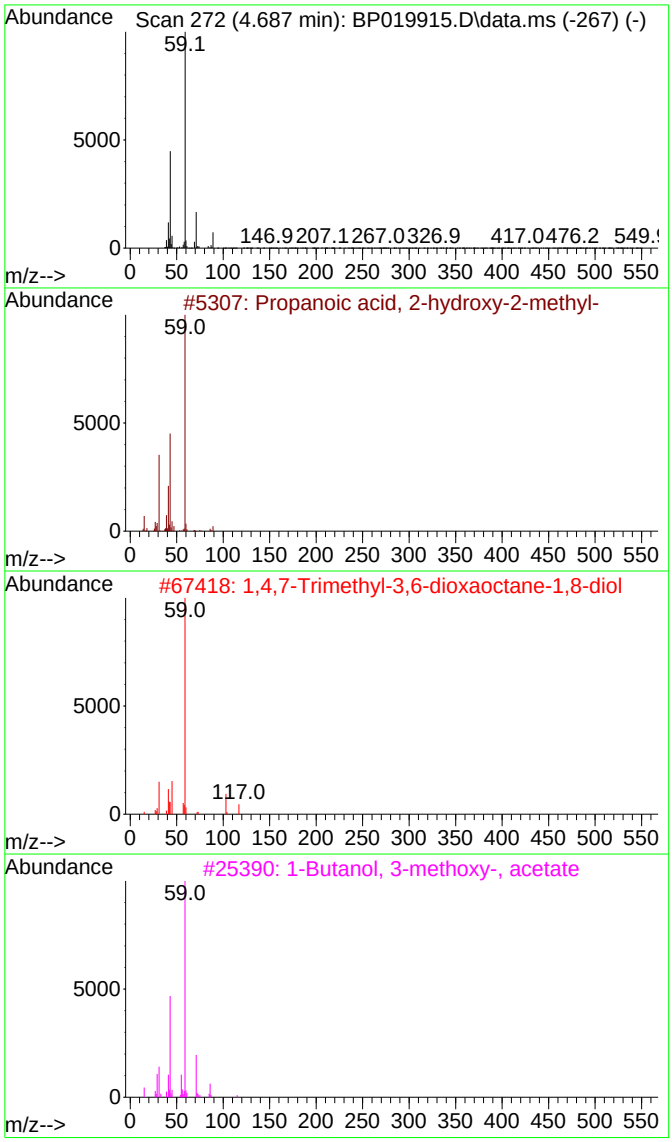
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

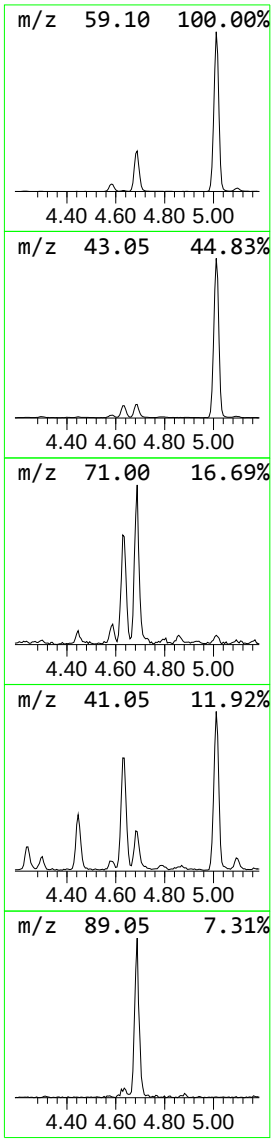
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, 2-hydroxy-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	8.19 ng	244667	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	50
2	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	42
3	1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	40
4	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	39
5	1-(1-Methoxypropan-2-yloxy)propa...	244	C9H15F3O4	1010367-08-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

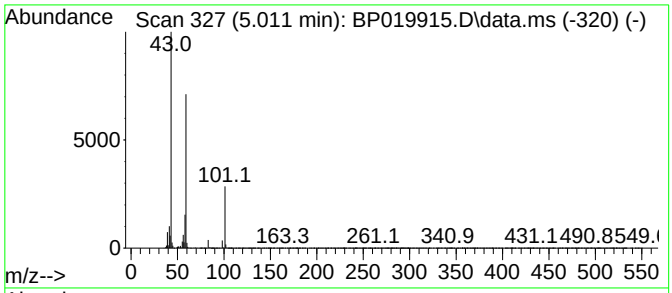
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

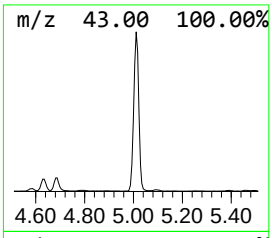
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

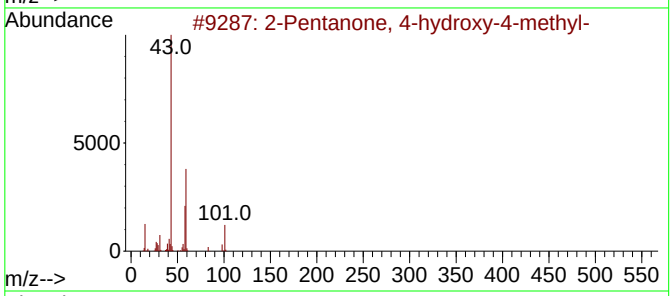
****
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

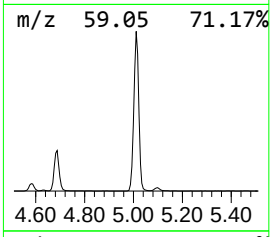
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	50.80 ng	1518000	1,4-Dichlorobenzene-d4	7.887

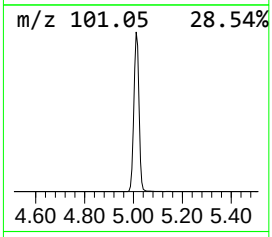
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25

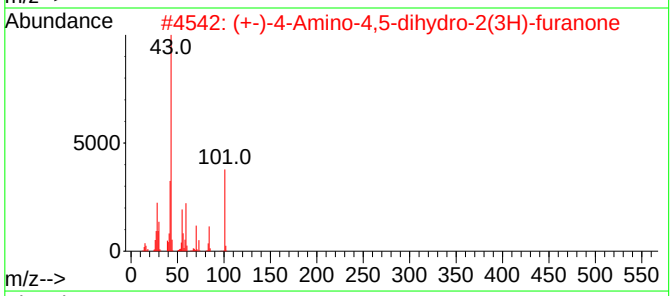


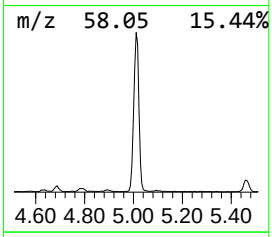


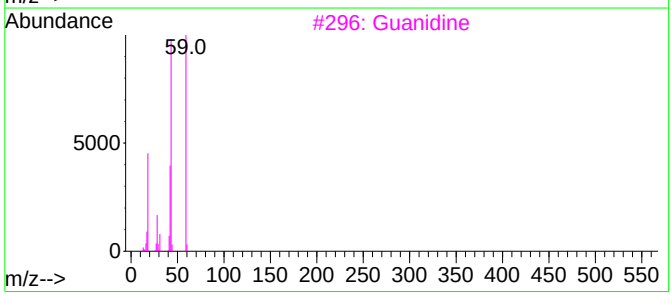


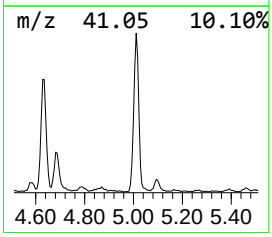












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

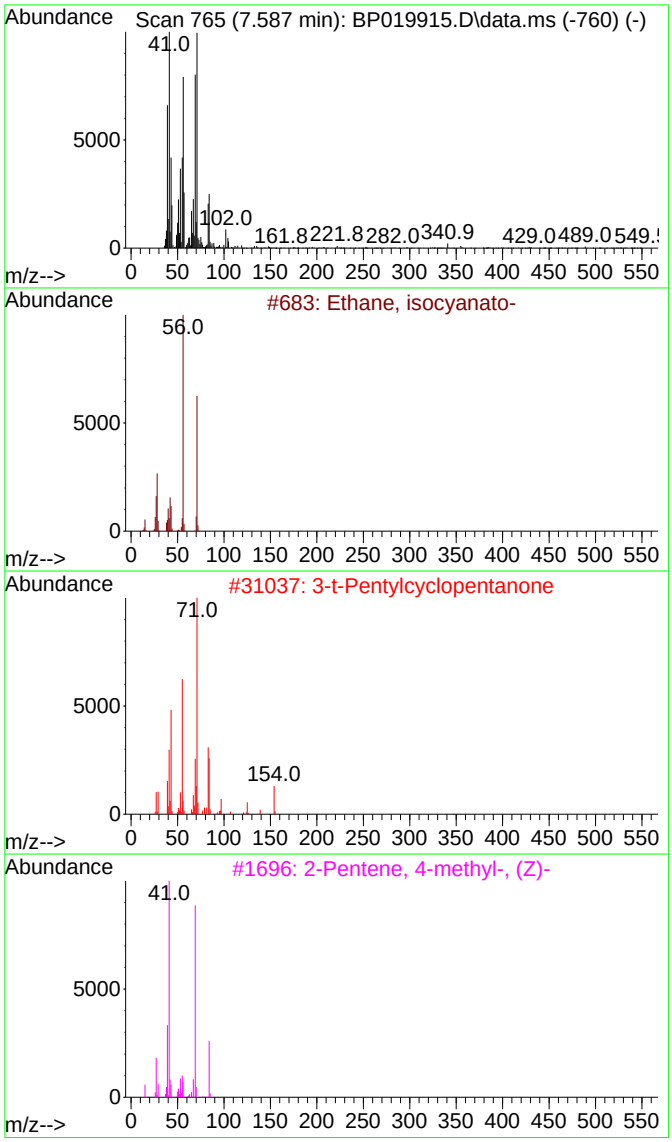
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

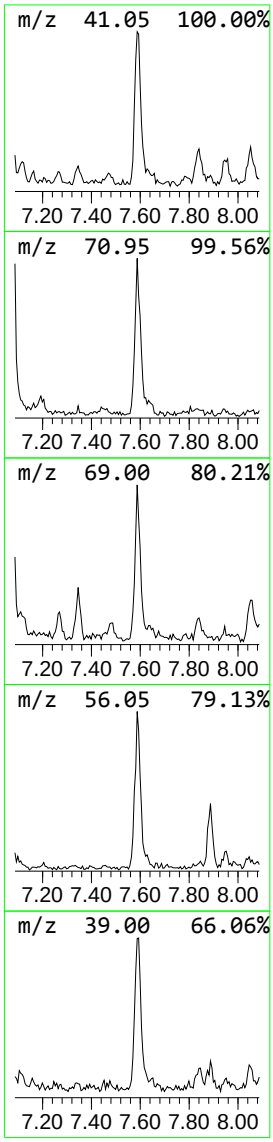
****

Peak Number 8 unknown7.587 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.587	4.23 ng	126513	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, isocyanato-	71	C3H5NO	000109-90-0	35
2	3-t-Pentylcyclopentanone	154	C10H18O	1000114-66-3	22
3	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	22
4	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	22
5	1-Hexene	84	C6H12	000592-41-6	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

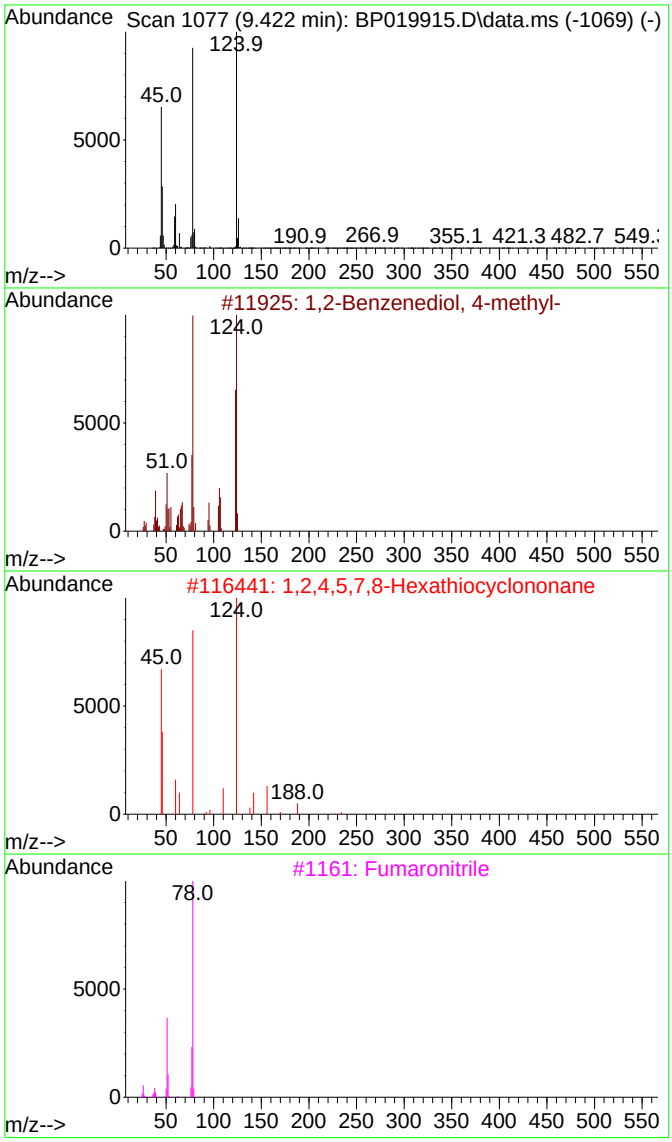
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

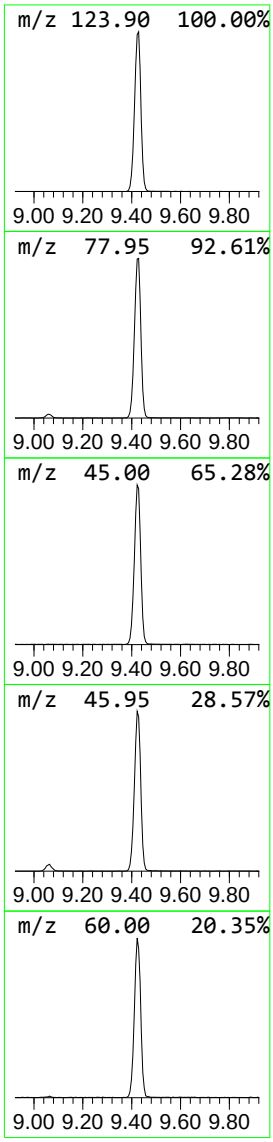
****

Peak Number 9 unknown9.422 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.422	59.44 ng	2357500	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
2	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	Benzene	78	C6H6	000071-43-2	9
5	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

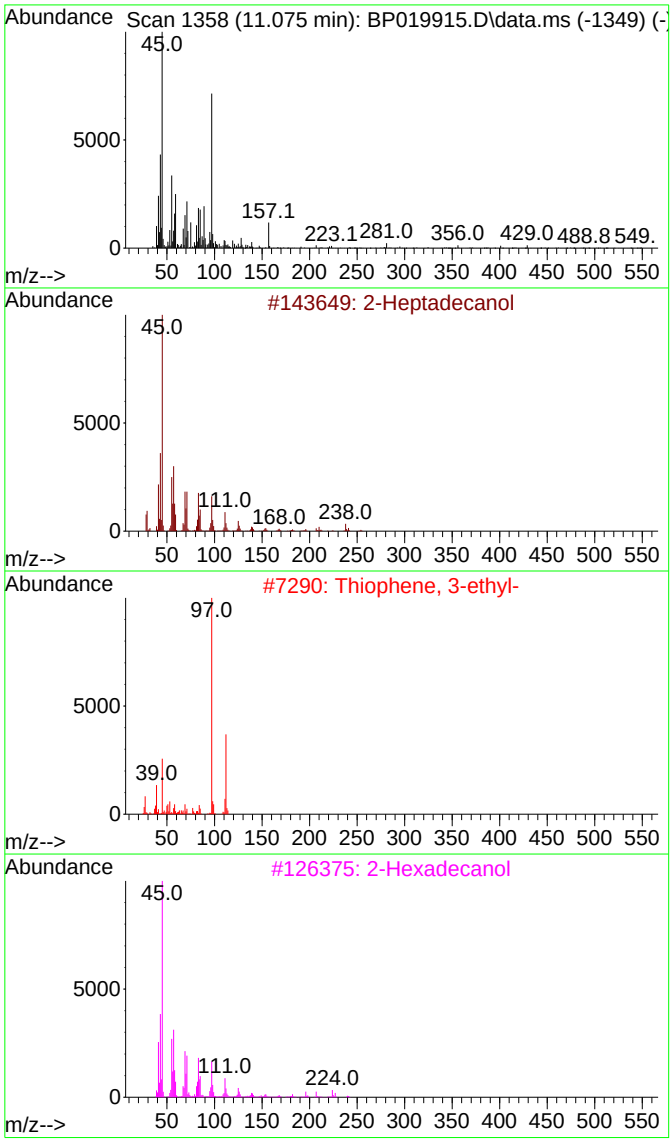
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

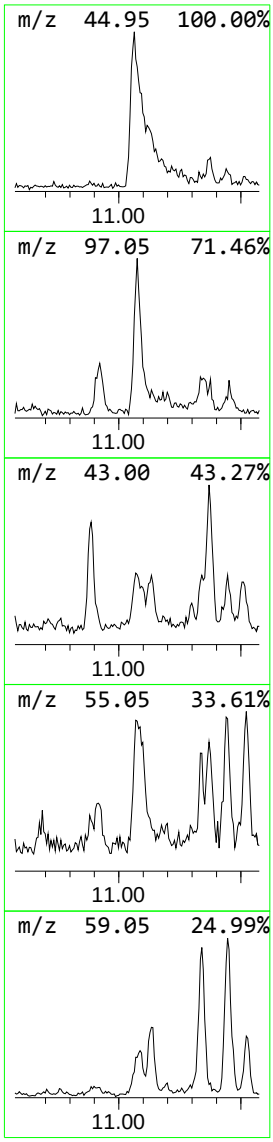
****

Peak Number 10 unknown11.075 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	3.33 ng	131954	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptadecanol	256	C17H36O	016813-18-6	49
2	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	47
3	2-Hexadecanol	242	C16H34O	014852-31-4	47
4	Triethylene glycol	150	C6H14O4	000112-27-6	38
5	2-Octene, 1-(methoxymethoxy)-, (E)-	172	C10H20O2	142509-32-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

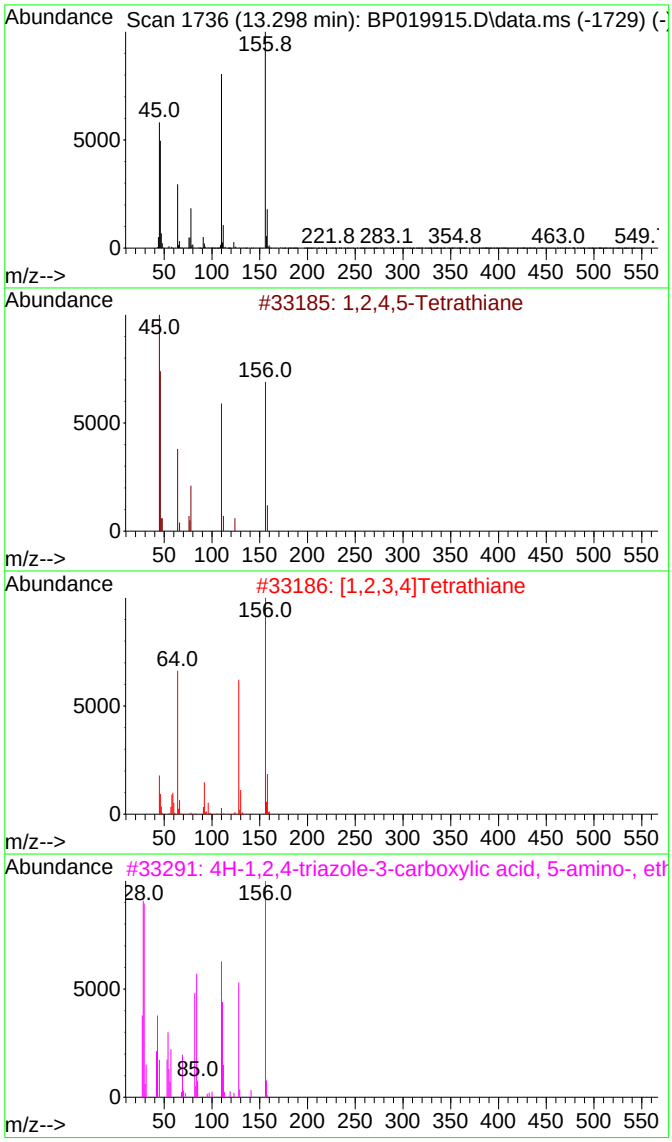
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

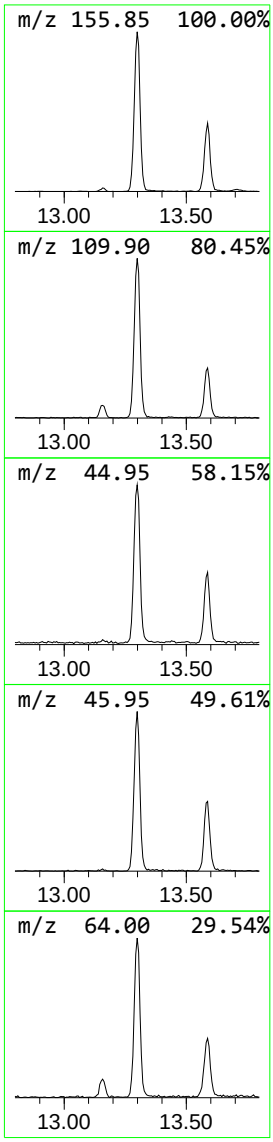
****

Peak Number 11 1,2,4,5-Tetrathiane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.299	6.44 ng	320489	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	78
2	[1,2,3,4]Tetrathiane	156	C2H4S4	000290-81-3	38
3	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	37
4	Omethoate	213	C5H12NO4PS	001113-02-6	28
5	2-Thiazolin-4-one, 2-(2-thienyl)-	183	C7H5NOS2	006114-95-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

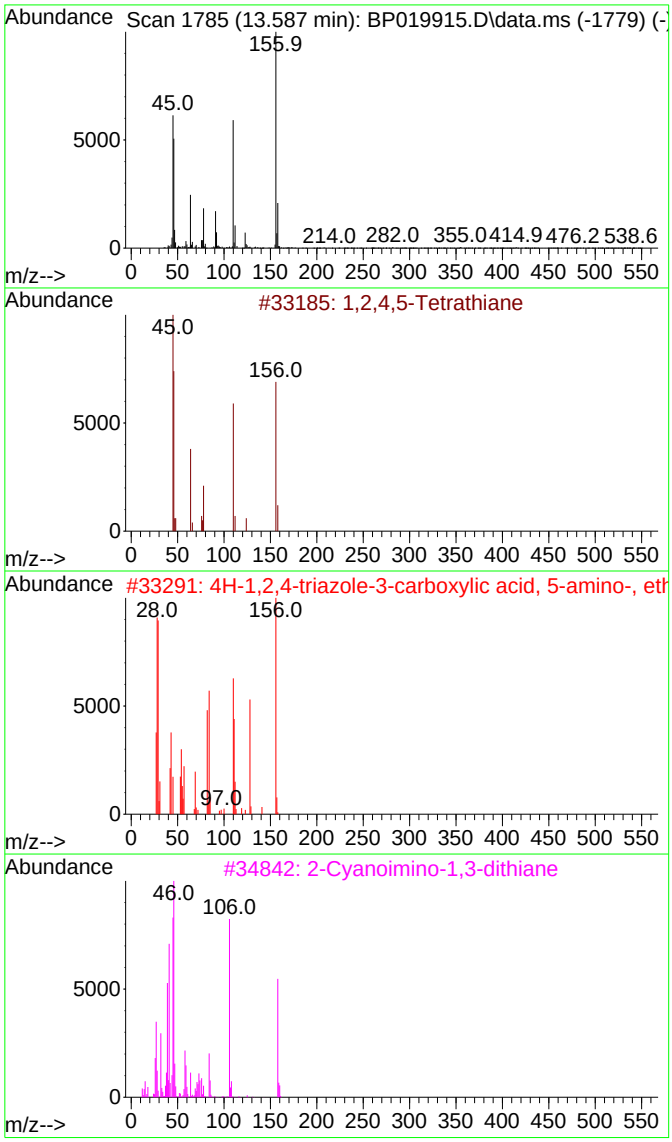
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

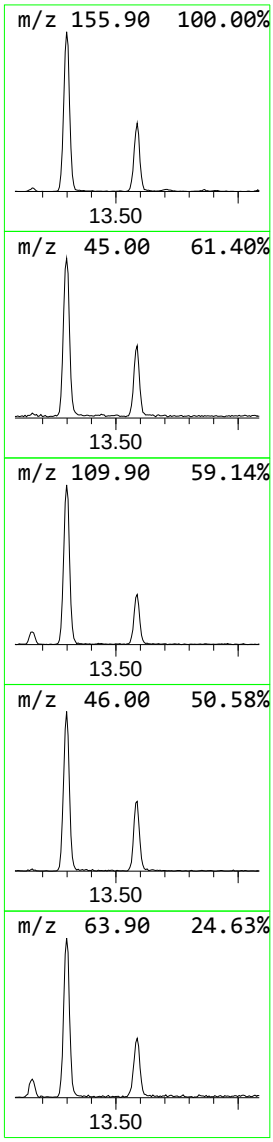
****

Peak Number 12 unknown13.587 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	2.81 ng	139643	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	90
2	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	38
3	2-Cyanoimino-1,3-dithiane	158	C5H6N2S2	010191-73-8	22
4	1-Aminocyclopentanecarboxylic ac...	229	C11H19NO4	1000328-97-0	10
5	2-Chloro-5-hydroxy-2,4,6-cyclohe...	156	C7H5ClO2	007009-16-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

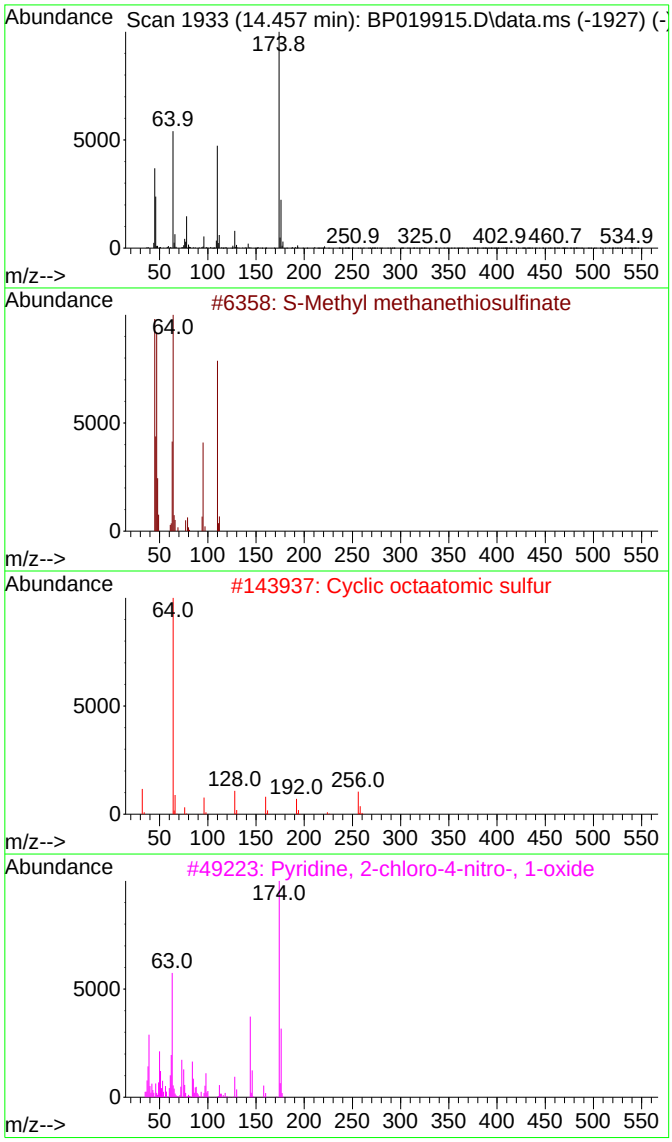
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

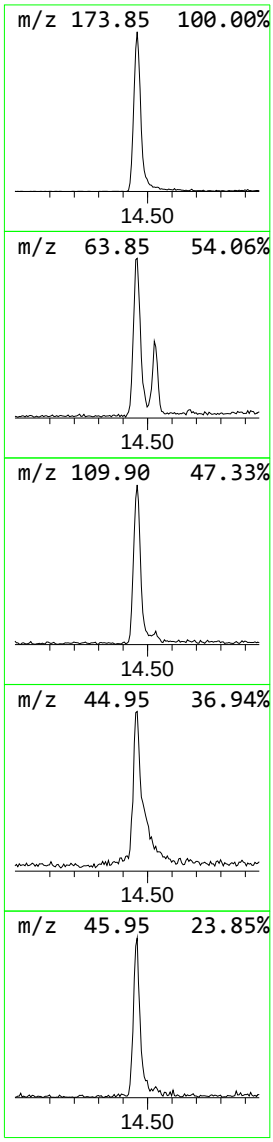
****

Peak Number 13 unknown14.457 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	3.38 ng	168071	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	40
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	17
3	Pyridine, 2-chloro-4-nitro-, 1-o...	174	C5H3ClN2O3	014432-16-7	10
4	3-Chloro-5-nitro-2(1H)-pyridinone	174	C5H3ClN2O3	022353-38-4	9
5	3-Chloro-6-hydroxy-4-pyridazinec...	174	C5H3ClN2O3	061404-48-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

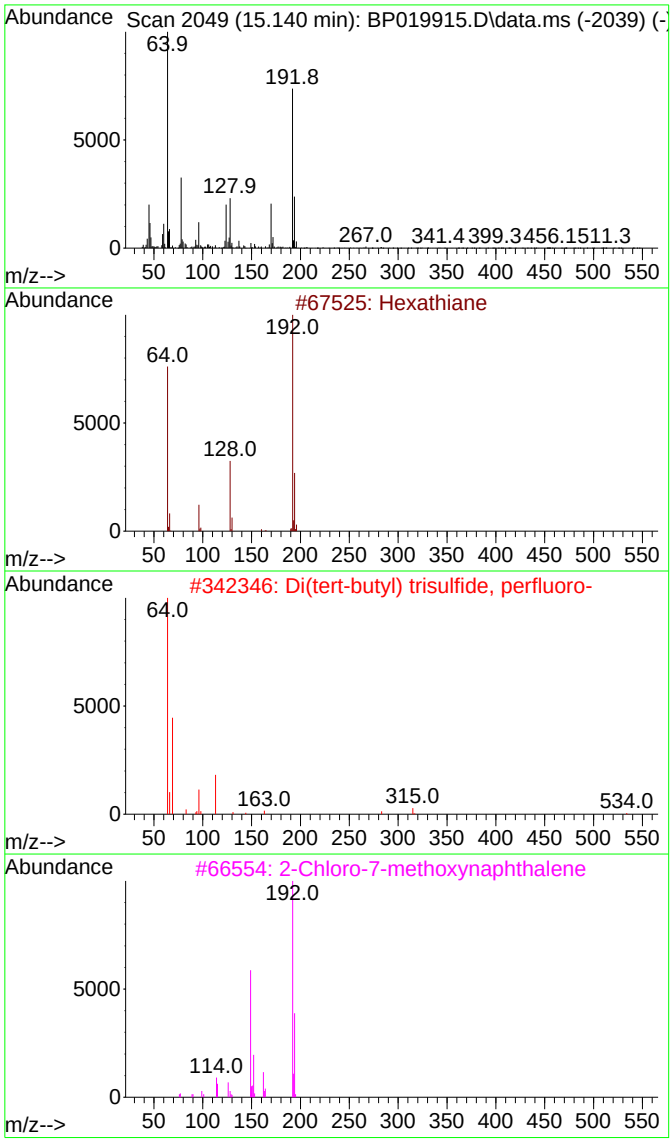
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

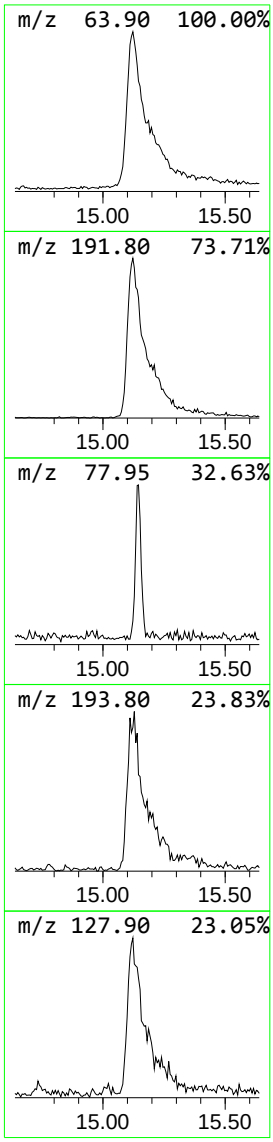
****

Peak Number 14 Hexathiane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.140	4.21 ng	209561	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	87
2	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	33
3	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	32
4	3-Methyl-4-chloro-1,2-dehydro-1-...	192	C7H10ClO2P	1000306-50-3	11
5	2(1H)-Quinoxalinone, 3-(methylth...	192	C9H8N2OS	1010338-35-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

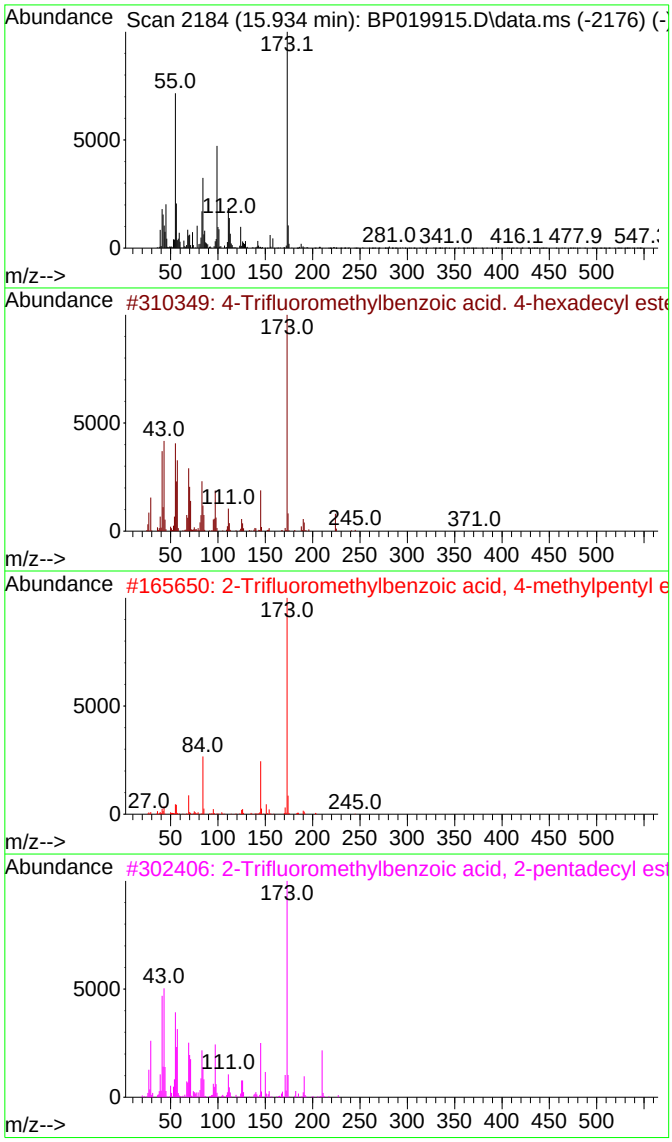
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

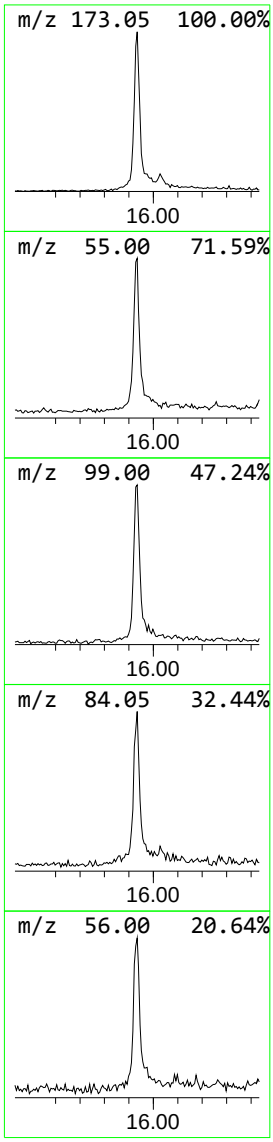
****

Peak Number 15 unknown15.934 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.934	5.05 ng	272916	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Trifluoromethylbenzoic acid. 4...	414	C24H37F3O2	1000283-03-4	43
2	2-Trifluoromethylbenzoic acid, 4...	274	C14H17F3O2	1000282-28-8	38
3	2-Trifluoromethylbenzoic acid, 2...	400	C23H35F3O2	1000282-03-5	38
4	2-Trifluoromethylbenzoic acid, 2...	246	C12H13F3O2	1010282-64-3	38
5	4,6-Dichloro-5-cyanopyrimidine	173	C5HCl2N3	005305-45-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

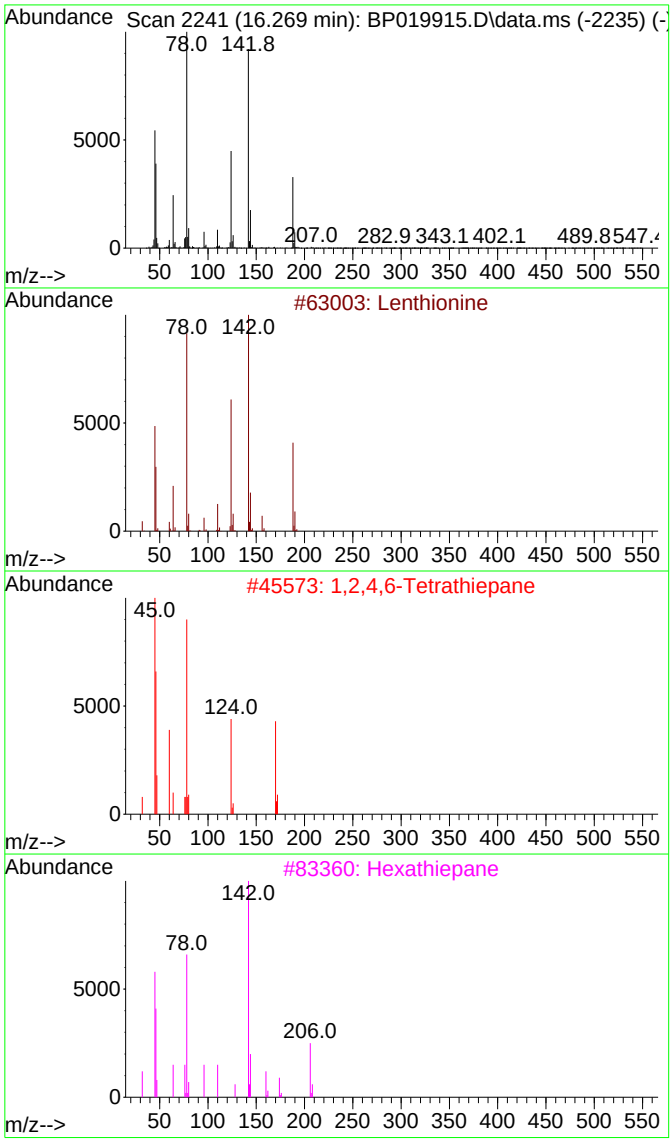
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

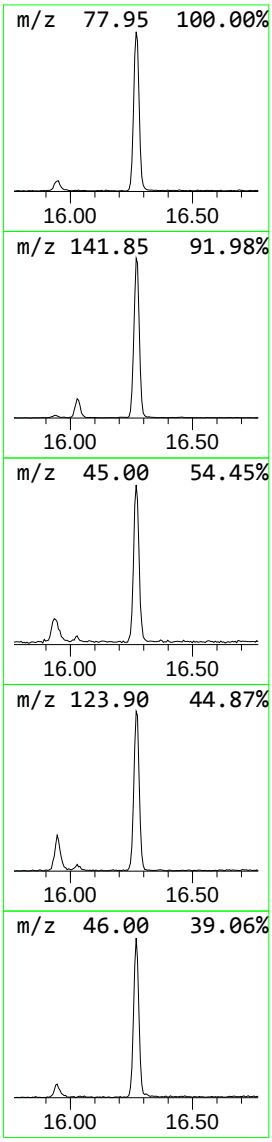
****

Peak Number 16 Lenthionine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	8.02 ng	433547	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	97
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3	Hexathiepane	206	CH2S6	017233-71-5	16
4	Fumaronitrile	78	C4H2N2	000764-42-1	9
5	Phenylphosphonous acid	142	C6H7O2P	001779-48-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

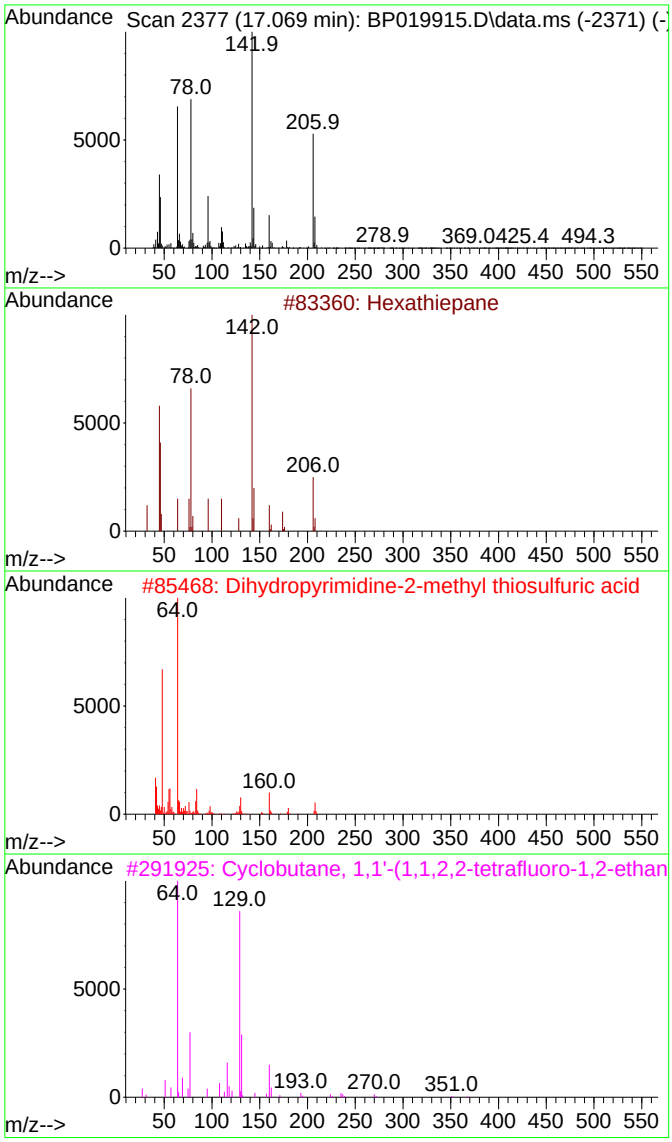
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

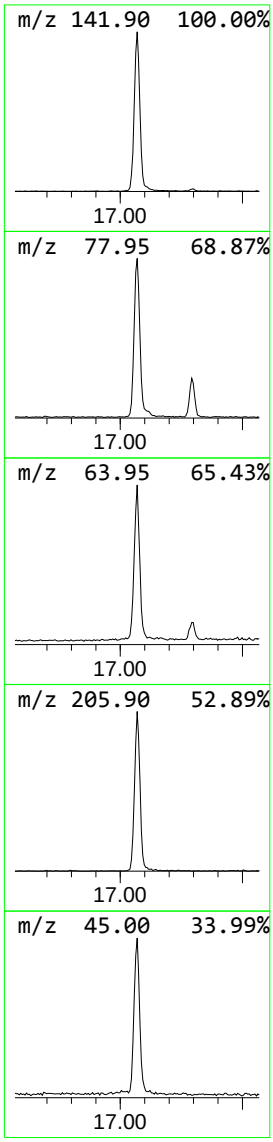
****

Peak Number 17 unknown17.069 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.069	10.76 ng	581474	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	17
2	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	12
3	Cyclobutane, 1,1'-(1,1,2,2-tetra...	386	C10H6Cl2F10	035208-02-7	12
4	1-Aminocyclopentanecarboxylic ac...	411	C24H45NO4	1000328-91-0	10
5	1,3-Benzenedithiol	142	C6H6S2	000626-04-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

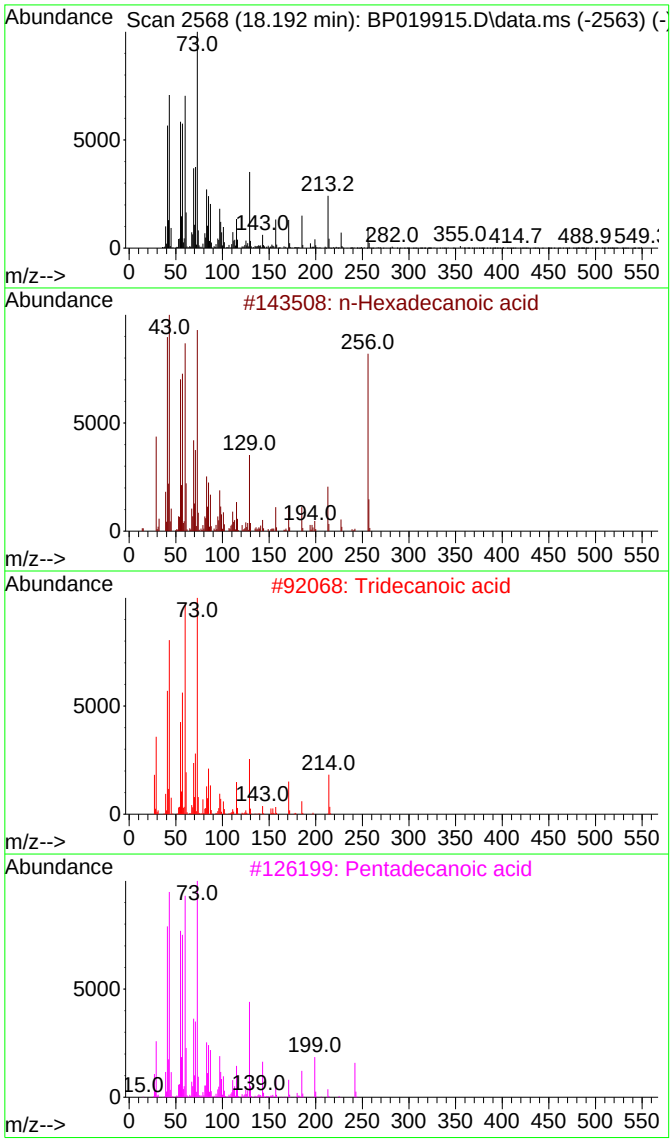
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

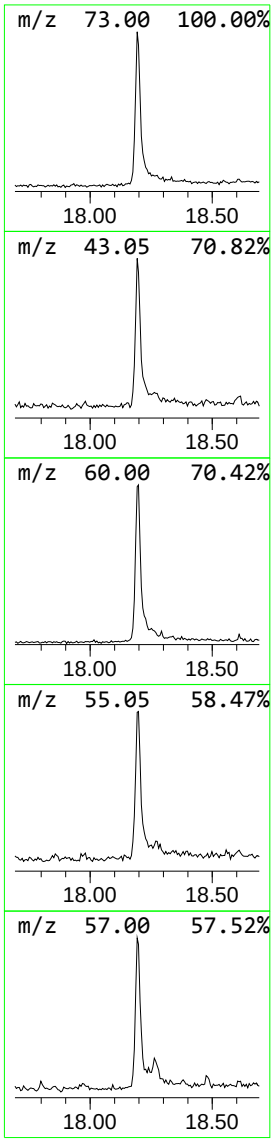
****

Peak Number 18 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	7.84 ng	423925	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
5	Octadecanoic acid	284	C18H36O2	000057-11-4	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

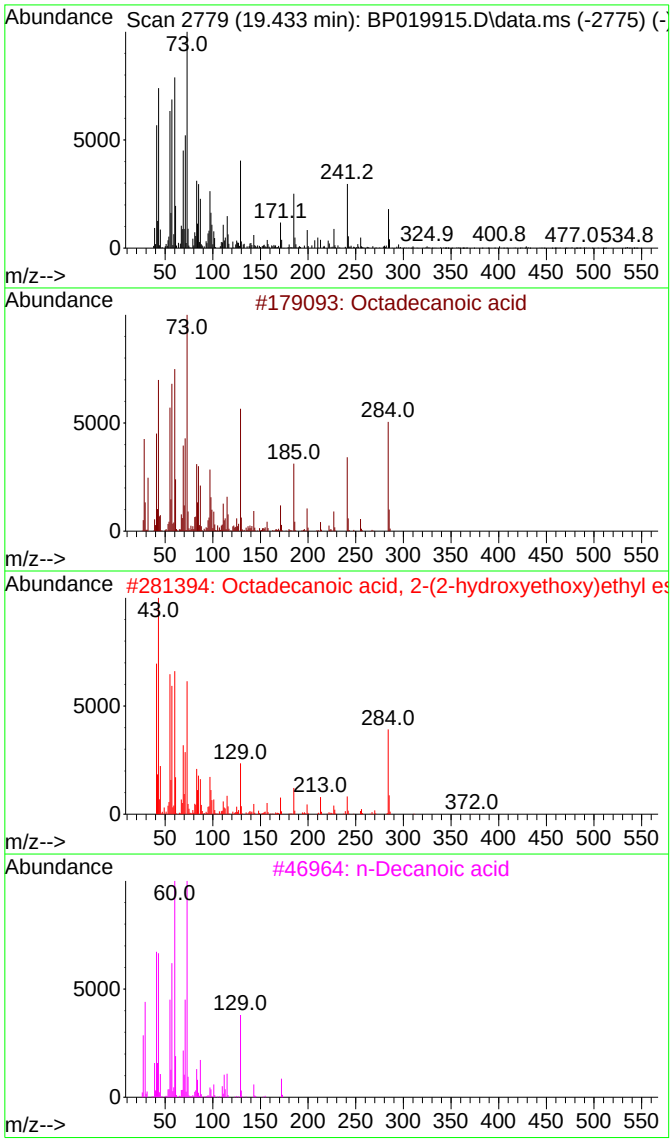
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

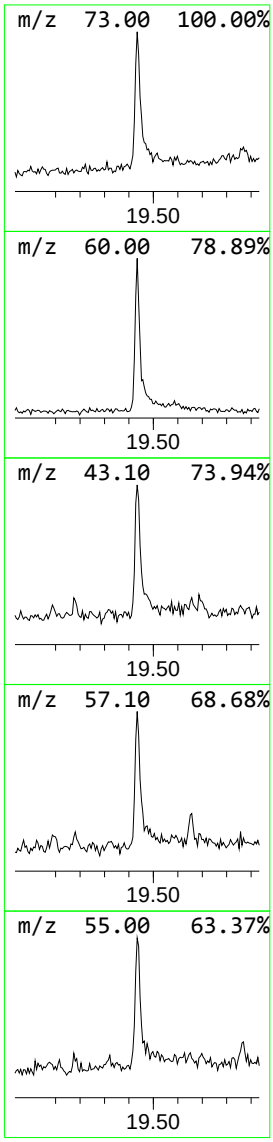
****

Peak Number 19 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	3.68 ng	239539	Chrysene-d12	21.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

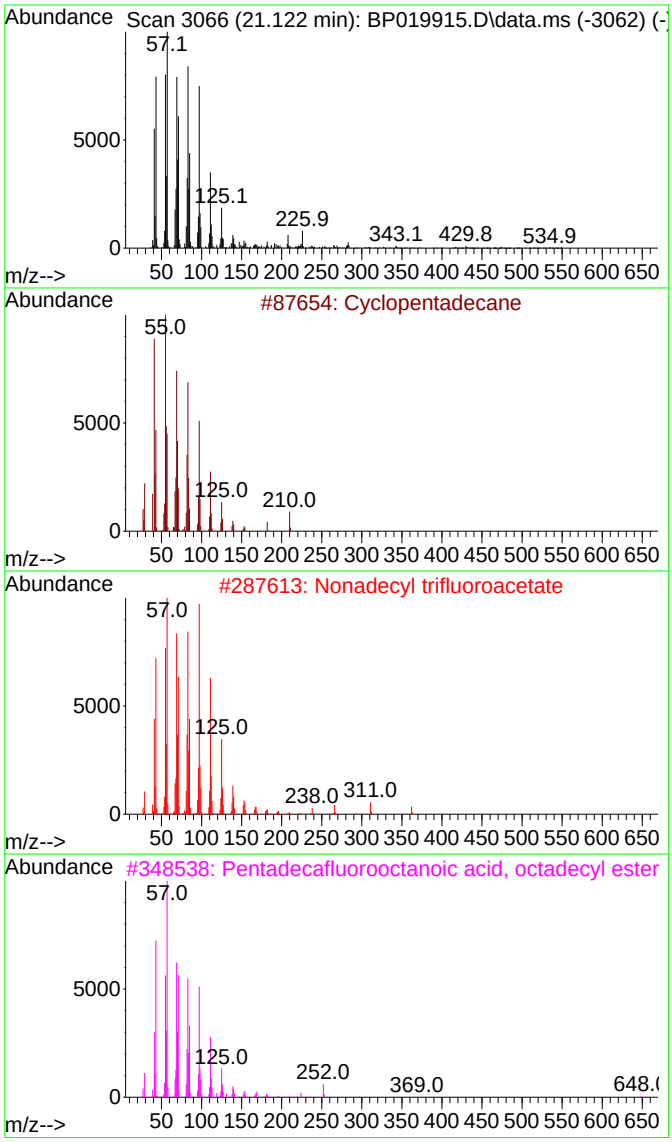
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

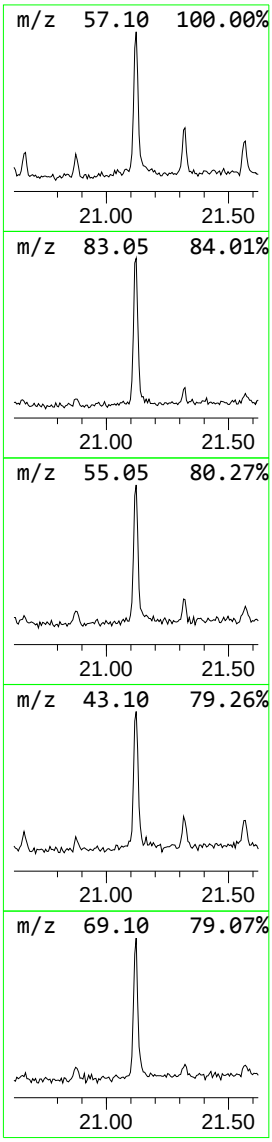
****

Peak Number 20 Cyclopentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	4.61 ng	299978	Chrysene-d12	21.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Heptacos-1-ene	378	C27H54	015306-27-1	90
5	1-Tetracosene	336	C24H48	010192-32-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022824\
Data File : BP019915.D
Acq On : 28 Feb 2024 14:21
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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	97.8	ng	2923870	1	7.887	597653	20.0
Prenol	4.064	9.7	ng	289015	1	7.887	597653	20.0
2-Butenal, 3-me...	4.234	2.9	ng	85904	1	7.887	597653	20.0
3-Hexen-1-ol	4.446	3.3	ng	98755	1	7.887	597653	20.0
2-Pentanol, 4-m...	4.634	13.2	ng	394490	1	7.887	597653	20.0
Propanoic acid,...	4.687	8.2	ng	244667	1	7.887	597653	20.0
2-Pentanone, 4-...	5.011	50.8	ng	1518000	1	7.887	597653	20.0
unknown7.587	7.587	4.2	ng	126513	1	7.887	597653	20.0
unknown9.422	9.422	59.4	ng	2357500	2	10.687	793302	20.0
unknown11.075	11.075	3.3	ng	131954	2	10.687	793302	20.0
1,2,4,5-Tetrath...	13.299	6.4	ng	320489	3	14.534	994721	20.0
unknown13.587	13.587	2.8	ng	139643	3	14.534	994721	20.0
unknown14.457	14.457	3.4	ng	168071	3	14.534	994721	20.0
Hexathiane	15.140	4.2	ng	209561	3	14.534	994721	20.0
unknown15.934	15.934	5.0	ng	272916	4	17.292	1080940	20.0
Lenthionine	16.269	8.0	ng	433547	4	17.292	1080940	20.0
unknown17.069	17.069	10.8	ng	581474	4	17.292	1080940	20.0
n-Hexadecanoic ...	18.192	7.8	ng	423925	4	17.292	1080940	20.0
Octadecanoic acid	19.433	3.7	ng	239539	5	21.398	1301650	20.0
Cyclopentadecane	21.122	4.6	ng	299978	5	21.398	1301650	20.0