LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4

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_F\Methods\8270-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140438.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	22	33	rVB	27275	47740	2.65%	0.298%
2	3.405	219	223	242	rBV	5128	19865	1.10%	0.124%
3	4.528	407	414	420	rVB4	11765	24626	1.37%	0.154%
4	4.934	474	483	488	rBV3	11583	18926	1.05%	0.118%
5	5.004	488	495	498	rVV4	27588	50838	2.82%	0.317%
6	5.034	498	500	504	rVV	16648	23533	1.31%	0.147%
7	5.087	504	509	515	rVV2	74814	121767	6.76%	0.760%
8	5.293	538	544	551	rBV	66702	118922	6.60%	0.743%
9	5.357	551	555	559	rVV2	51288	85572	4.75%	0.534%
10	5.393	559	561	566	rVV	26237	34516	1.92%	0.216%
11	5.469	566	574	575	rVV2	182697	261821	14.53%	1.635%
12	5.498	575	579	587	rVV	1119160	1544709	85.75%	9.646%
13	5.569	587	591	595	rVV	45908	66983	3.72%	0.418%
14	5.616	595	599	601	rVV2	17267	26194	1.45%	0.164%
15	5.651	601	605	608	rVV3	41848	72175	4.01%	0.451%
16	5.693	608	612	614	rVV	56268	77116	4.28%	0.482%
17	5.722	614	617	623	rVV2	86090	135500	7.52%	0.846%
18	5.781	623	627	638	rVB	126293	171567	9.52%	1.071%
19	5.898	638	647	651	rBV3	51682	92377	5.13%	0.577%
20	5.940	651	654	662	rVV4	13576	24817	1.38%	0.155%
21	6.034	664	670	674	rVB3	25897	41127	2.28%	0.257%
22	6.122	679	685	691	rBV4	53424	97552	5.42%	0.609%
23	6.310	712	717	720	rBV3	20737	31469	1.75%	0.197%
24	6.369	720	727	729	rVV3	22638	38228	2.12%	0.239%
25	6.404	729	733	739	rVB3	35138	54010	3.00%	0.337%
26	6.510	745	751	760	rBV	1179380	1560267	86.61%	9.743%
27	6.610	764	768	772	rBV3	22670	37960	2.11%	0.237%
28	6.704	780	784	791	rBV	117373	159786	8.87%	0.998%
29	6.875	807	813	818	rVB	598920	769640	42.72%	4.806%
30	7.016	833	837	841	rBV3	36322	45060	2.50%	0.281%
31	7.140	853	858	861	rBV5	22983	32798	1.82%	0.205%
32	7.257	873	878	883	rBV2	18964	35241	1.96%	0.220%
33	7.434	897	908	912	rBV	722722	993080	55.13%	6.202%
34	7.510	917	921	926	rVB5	10956	18634	1.03%	0.116%
35	7.681	946	950	957	rVB2	16776	25094	1.39%	0.157%
36	8.151	1022	1030	1043	rBV	719035	958896	53.23%	5.988%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4

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_F\Methods\8270-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.228	1207	1213	1223	rBV	1352807	1801466	100.00%	11.250%
38	9.910	1323	1329	1338	rBV	744755	980141	54.41%	6.121%
39	10.557	1430	1439	1444	rBV5	12826	26418	1.47%	0.165%
40	10.622	1445	1450	1456	rVV	250401	323349	17.95%	2.019%
41	10.698	1458	1463	1469	rVV	642121	835447	46.38%	5.217%
42	10.757	1469	1473	1479	rVV	29720	64728	3.59%	0.404%
43	10.810	1479	1482	1490	rVB2	18055	33780	1.88%	0.211%
44	10.933	1499	1503	1510	rVB	35638	49227	2.73%	0.307%
45	11.398	1576	1582	1591	rBV	676308	882469	48.99%	5.511%
46	11.922	1666	1671	1681	rBV2	76155	146006	8.10%	0.912%
47	12.086	1696	1699	1704	rBV5	13132	21249	1.18%	0.133%
48	12.616	1785	1789	1792	rBV	20298	32123	1.78%	0.201%
49	12.710	1802	1805	1808	rBV4	14854	20445	1.13%	0.128%
50	12.798	1817	1820	1823	rBV3	17755	20188	1.12%	0.126%
51	12.845	1825	1828	1835	rVV2	25672	43093	2.39%	0.269%
52	12.980	1846	1851	1859	rBV	1098621	1399137	77.67%	8.737%
53	13.463	1929	1933	1940	rVB	220838	294038	16.32%	1.836%
54	14.045	2028	2032	2039	rBV	475392	638795	35.46%	3.989%
55	15.551	2284	2288	2296	rVB	287552	483023	26.81%	3.016%

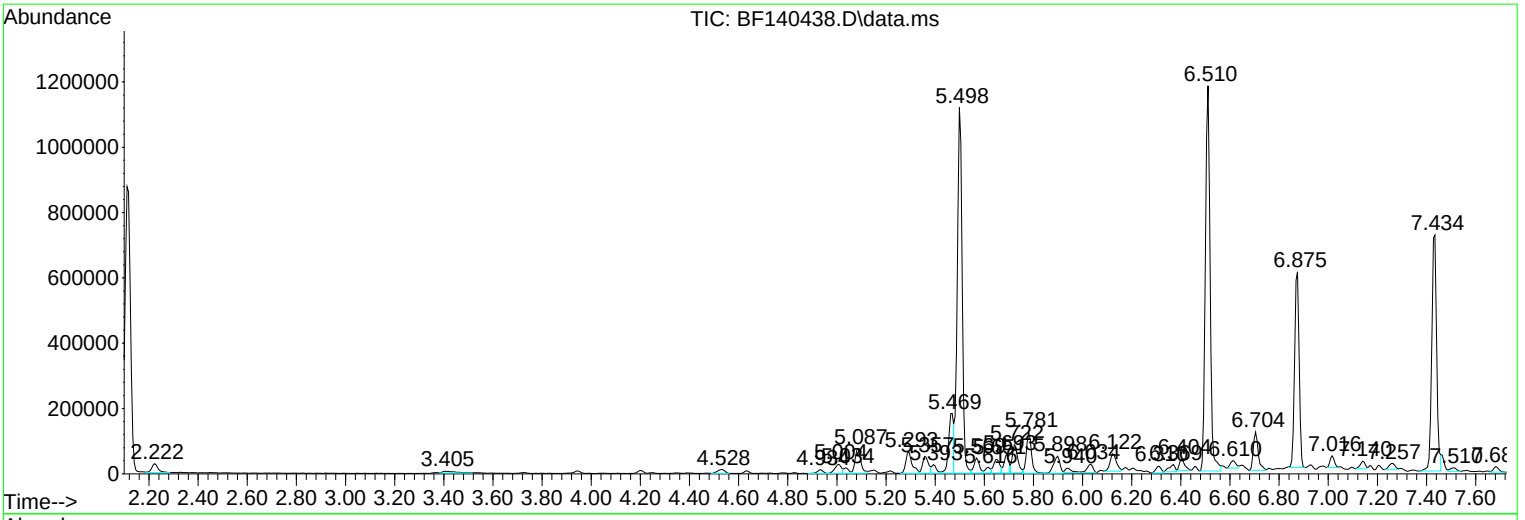
Sum of corrected areas: 16013528

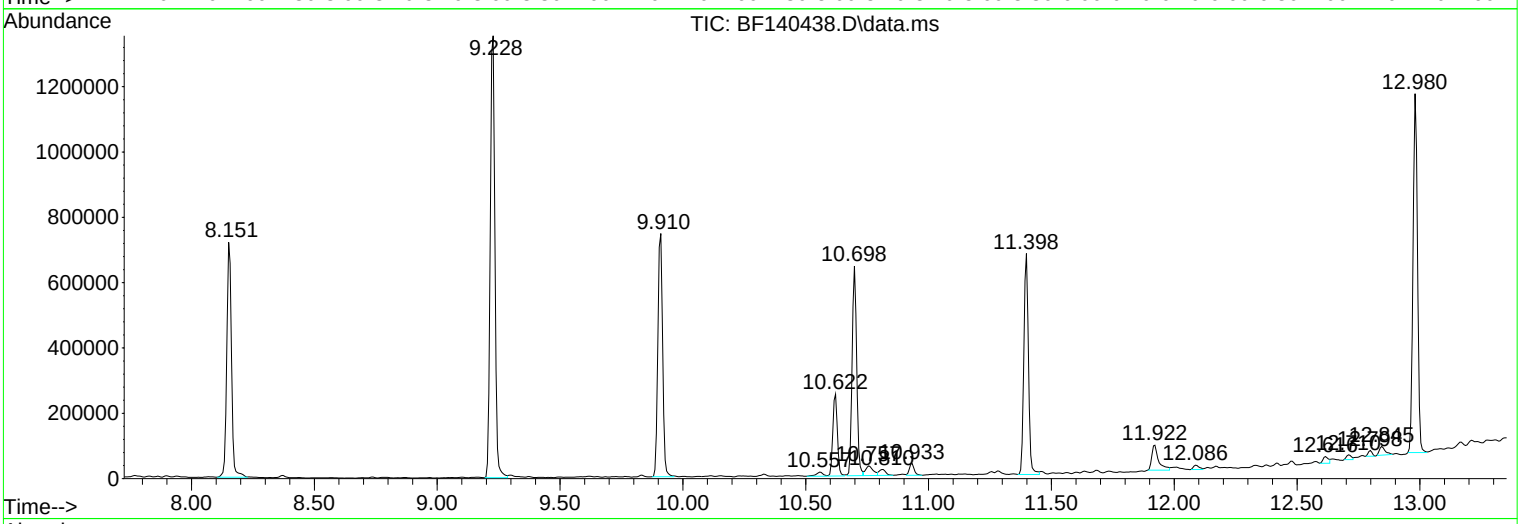
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

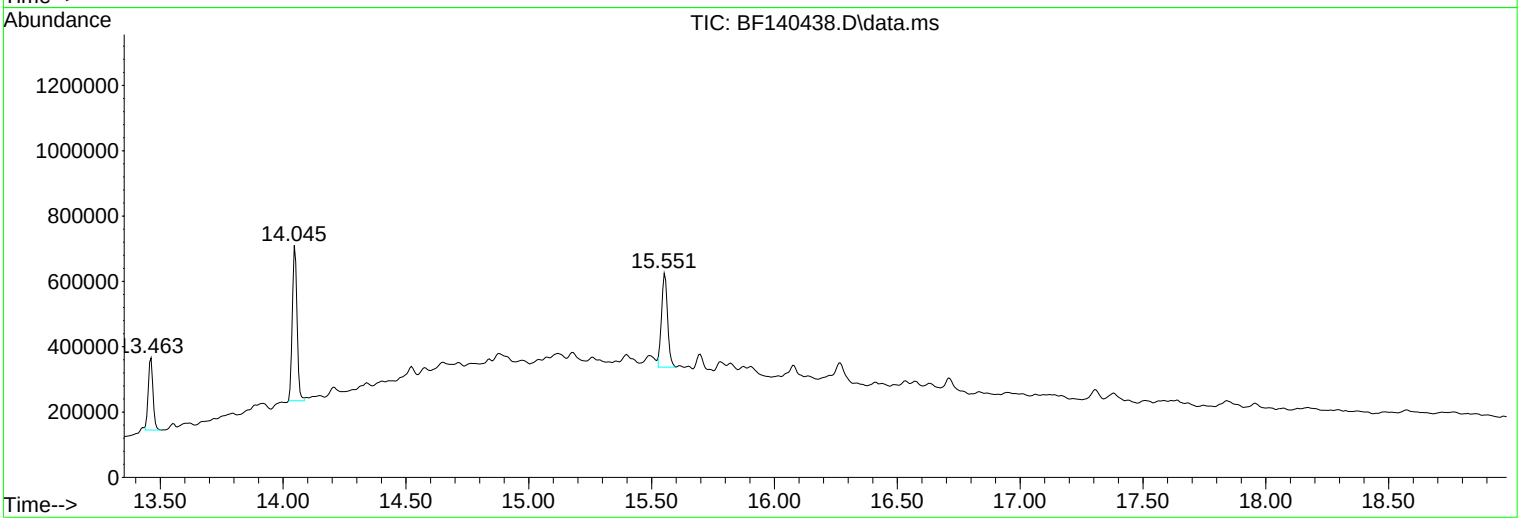
Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

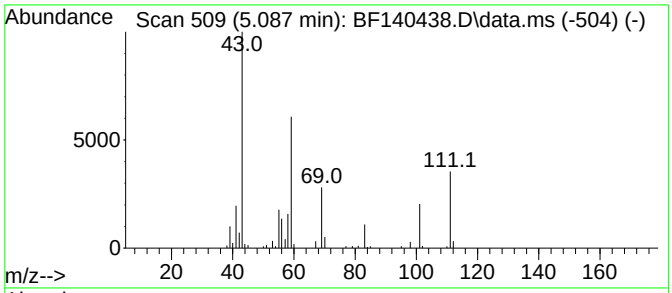
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

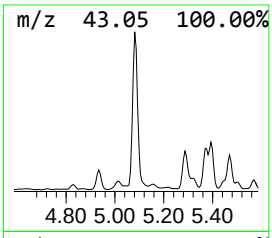
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

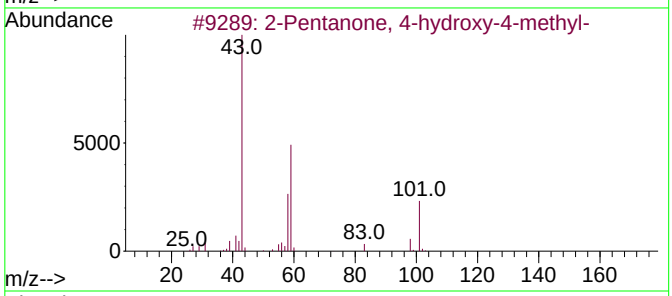
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

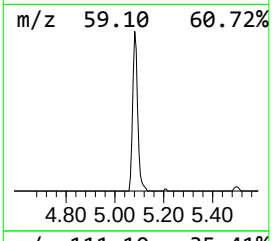
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	3.16 ng	121767	1,4-Dichlorobenzene-d4	6.875

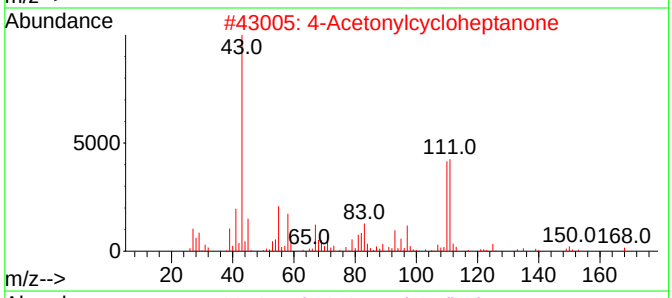
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	4-Acetonylcycloheptanone	168	C10H16O2	086428-60-6	17
3	1-(1,3-Oxazol-2-yl)ethan-1-one	111	C5H5NO2	077311-07-0	9
4	Acetone	58	C3H6O	000067-64-1	9
5	1-Heptyn-6-one	110	C7H10O	000928-39-2	9

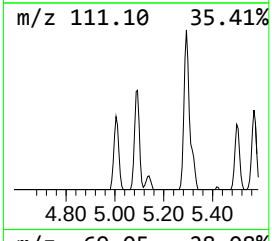


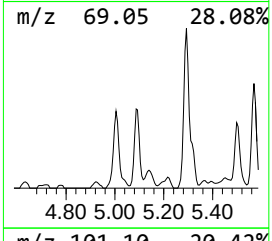


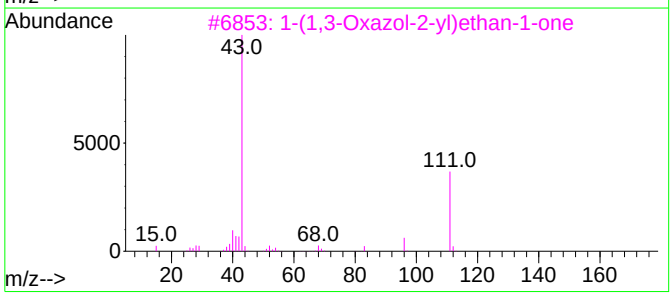


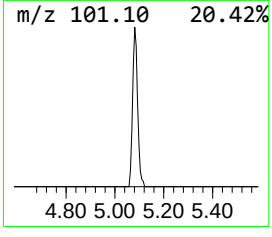












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

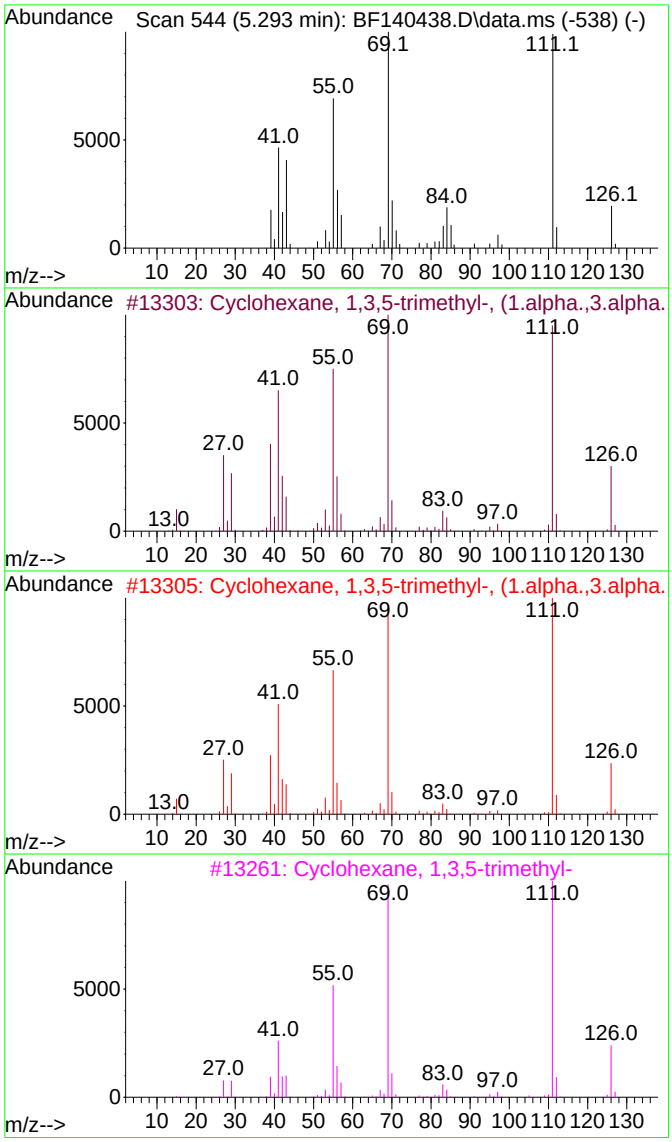
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

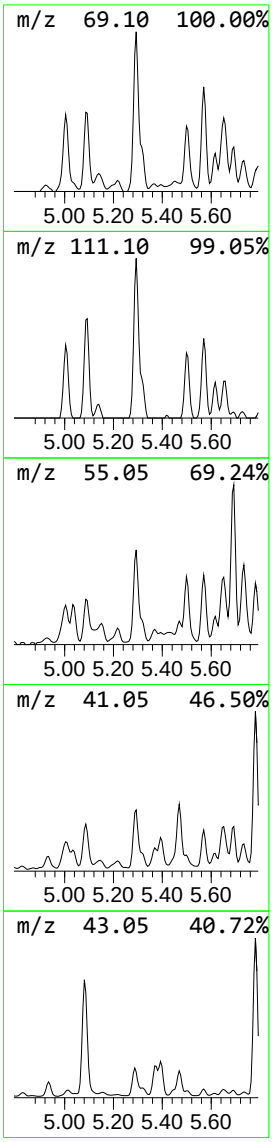
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,3,5-trimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.293	3.09 ng	118922	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	72
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
4	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	64
5	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

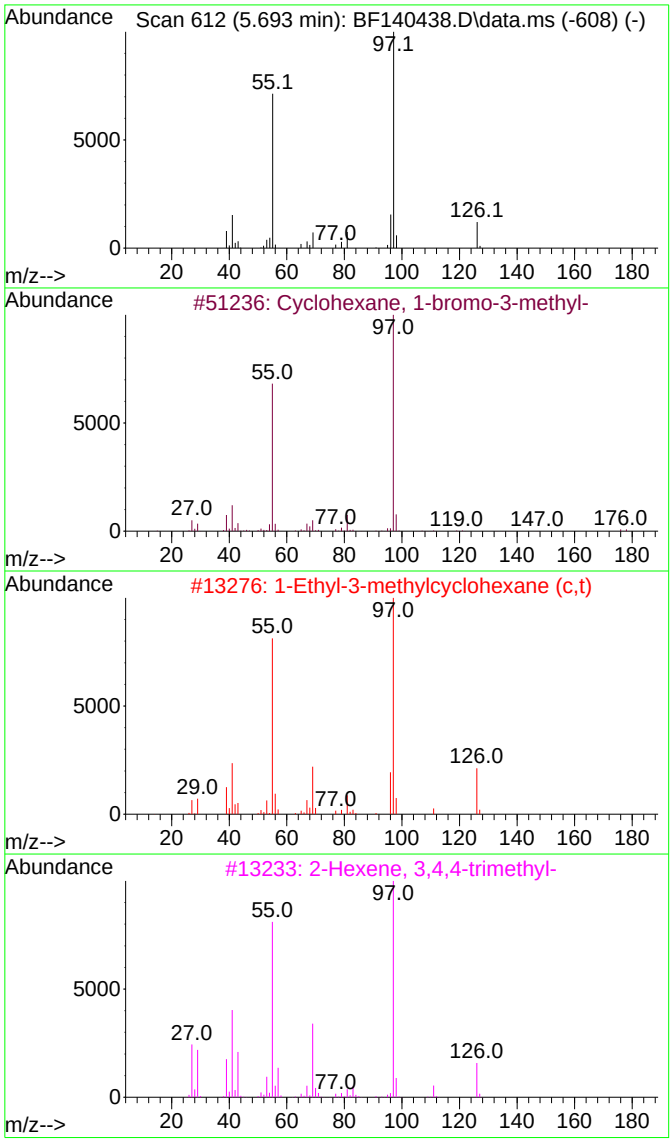
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

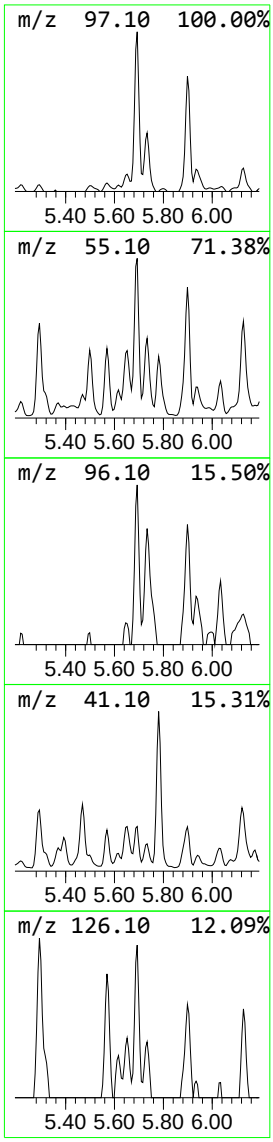
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexane, 1-bromo-3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.693	2.00 ng	77116	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-bromo-3-methyl-	176	C7H13Br	013905-48-1	64
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	64
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	64
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	64
5	Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

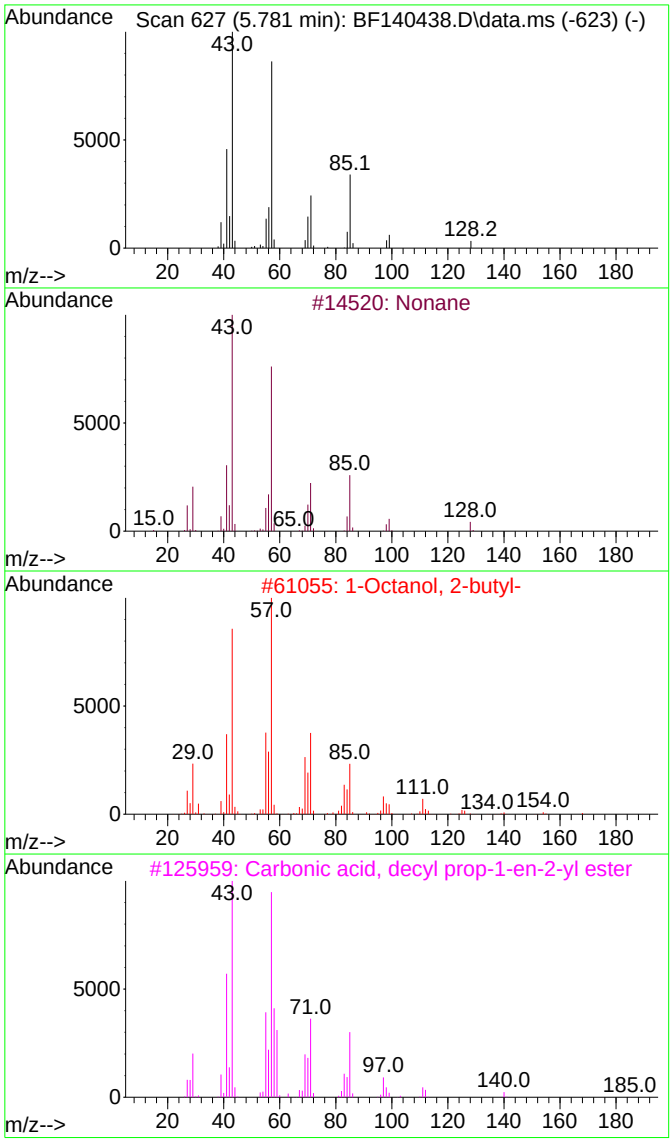
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

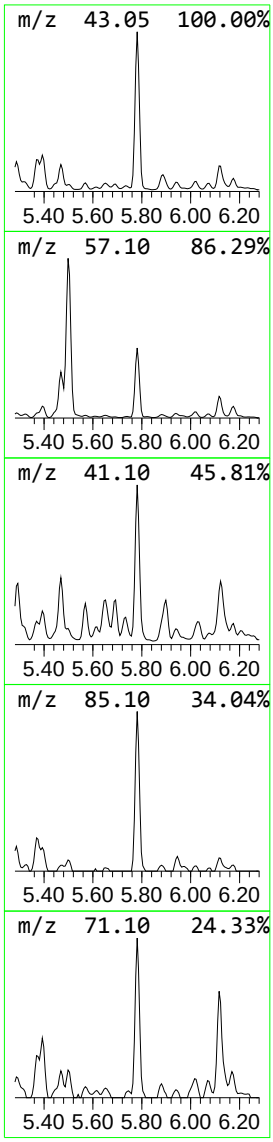
****

Peak Number 6 Nonane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.781	4.46 ng	171567	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	95
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	78
3	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	78
4	Octane	114	C8H18	000111-65-9	72
5	Octane, 4-methyl-	128	C9H20	002216-34-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

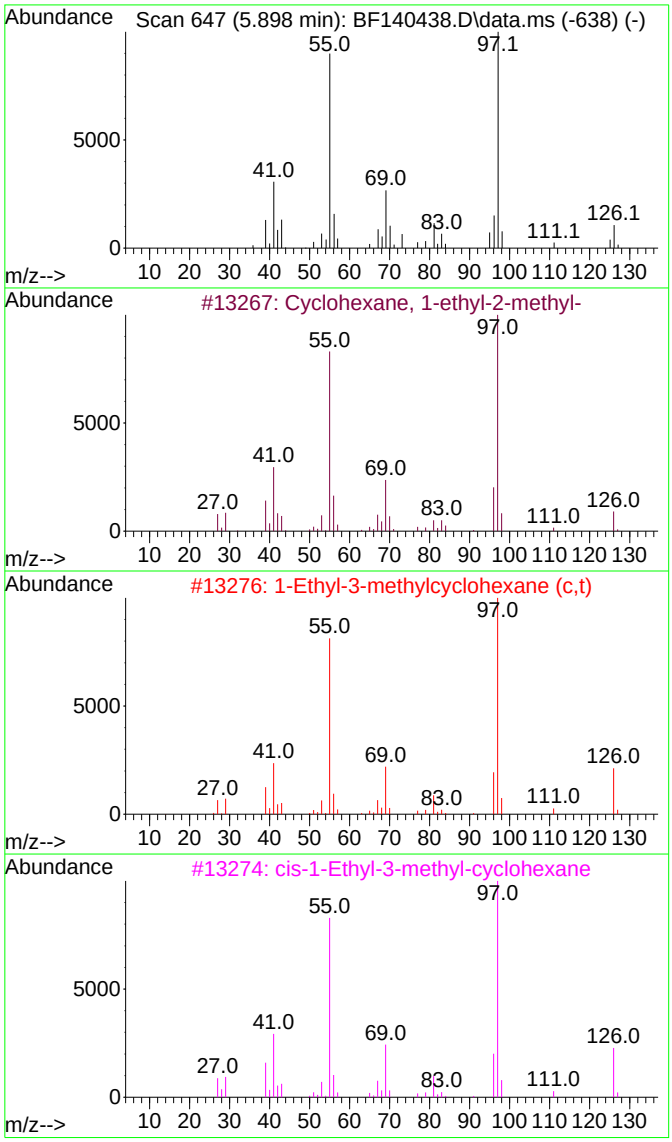
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

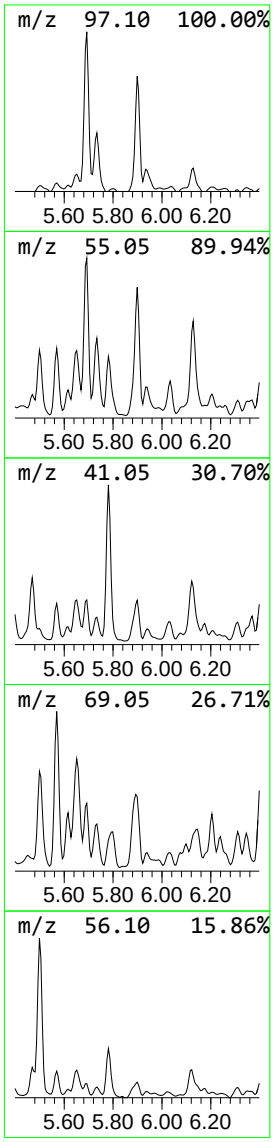
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.898	2.40 ng	92377	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	93
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	83
3	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	83
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

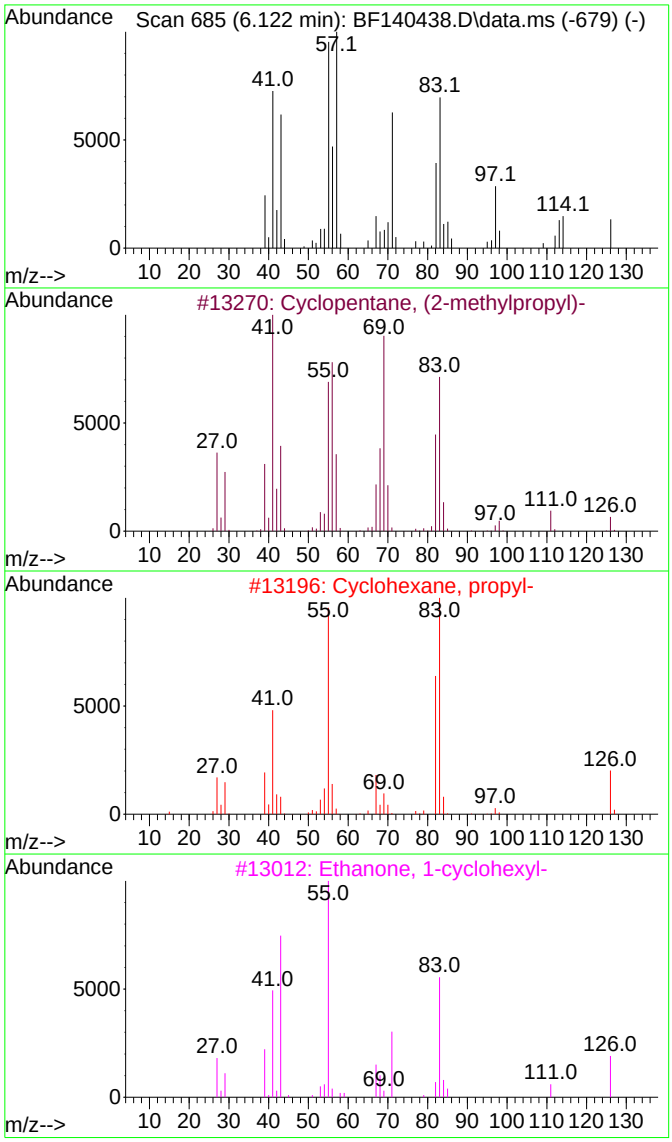
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

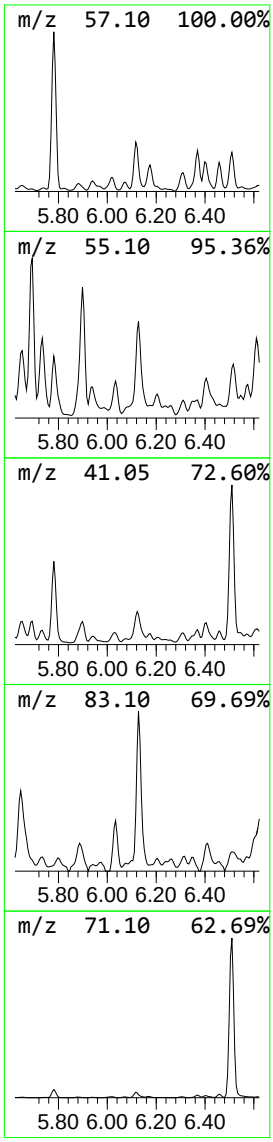
****

Peak Number 8 Cyclopentane, (2-methylprop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.122	2.54 ng	97552	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	53
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	38
3	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	30
4	Cyclopentane, butyl-	126	C9H18	002040-95-1	30
5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	27





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Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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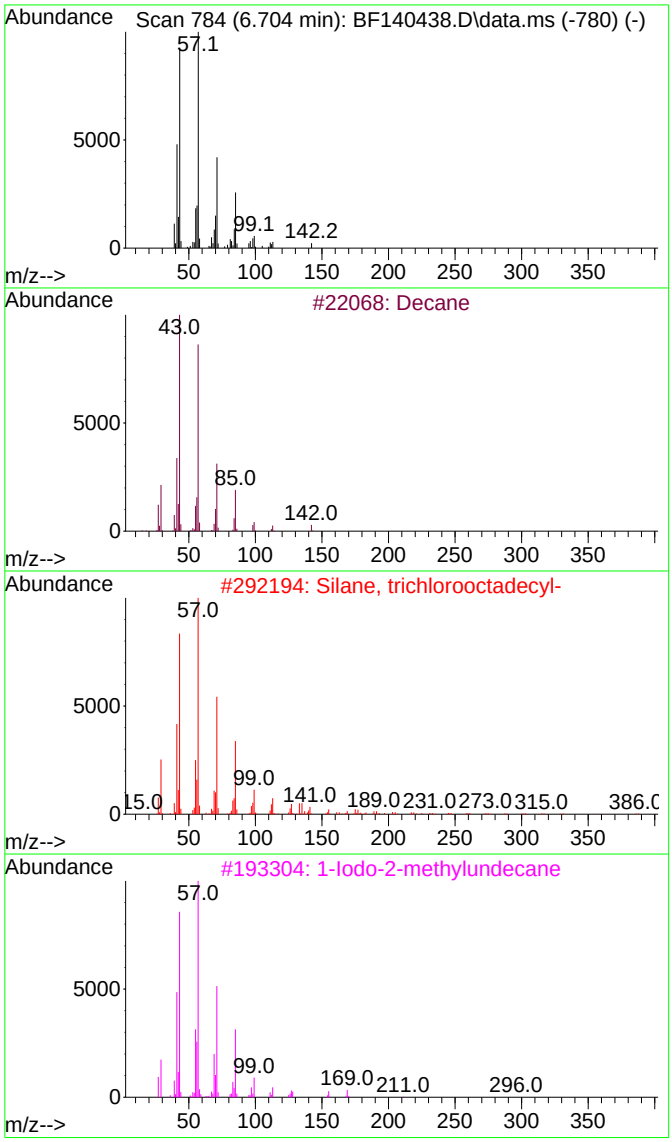
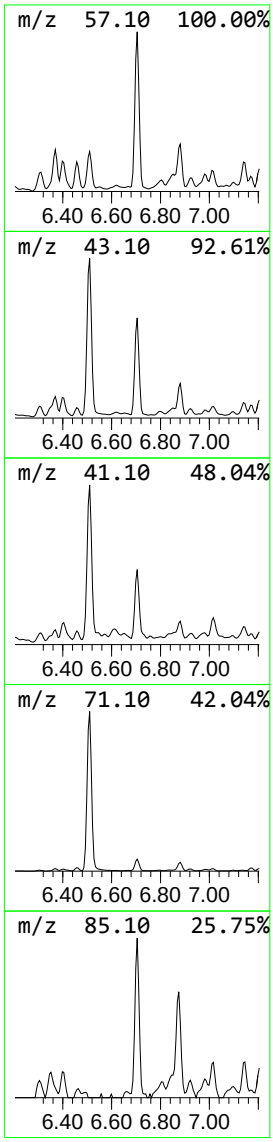
Peak Number 9 Decane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	4.15 ng	159786	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	95
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
4	Nonane	128	C9H20	000111-84-2	80
5	Tridecane	184	C13H28	000629-50-5	72





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Misc :
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BNA_F
ClientSampleId :
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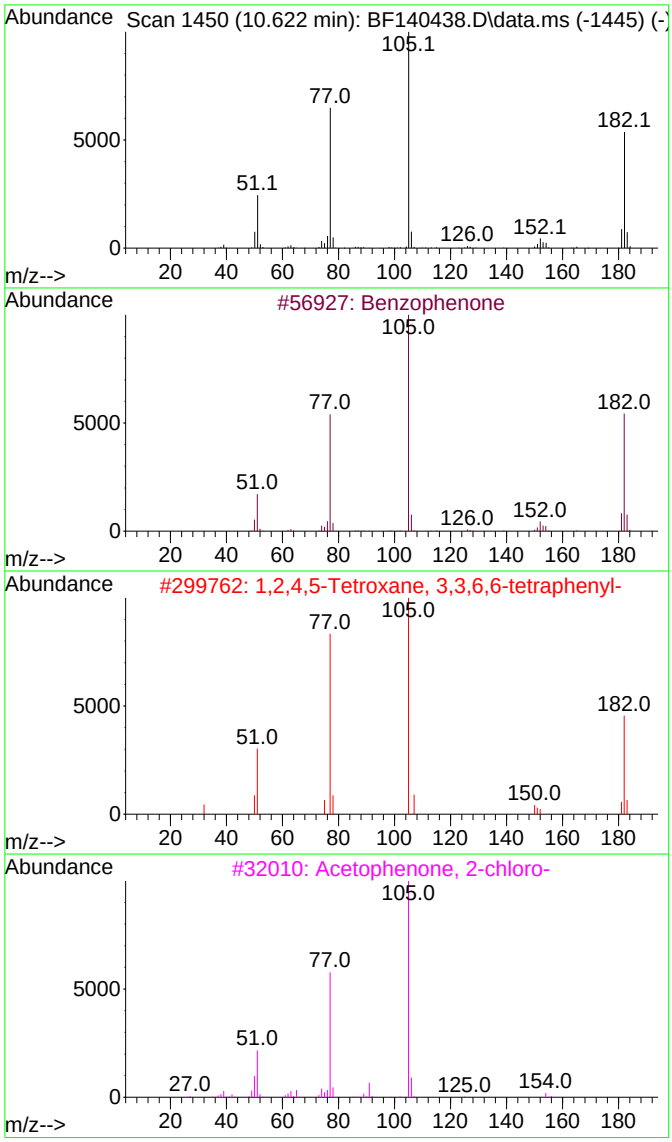
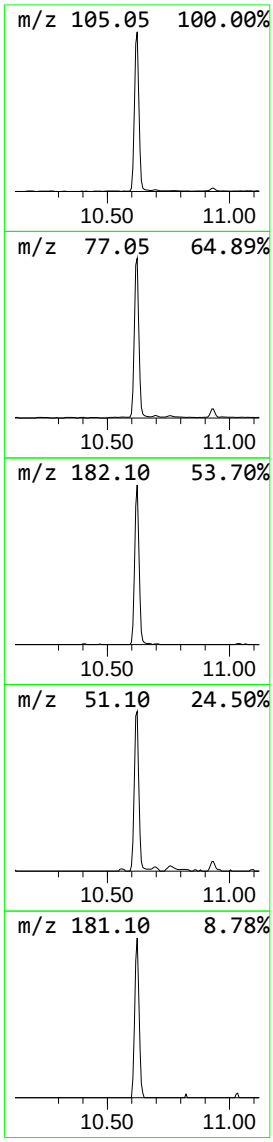
Peak Number 10 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	6.60 ng	323349	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





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Data File : BF140438.D
Acq On : 16 Nov 2024 18:53
Operator : RC/JU
Sample : P4768-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
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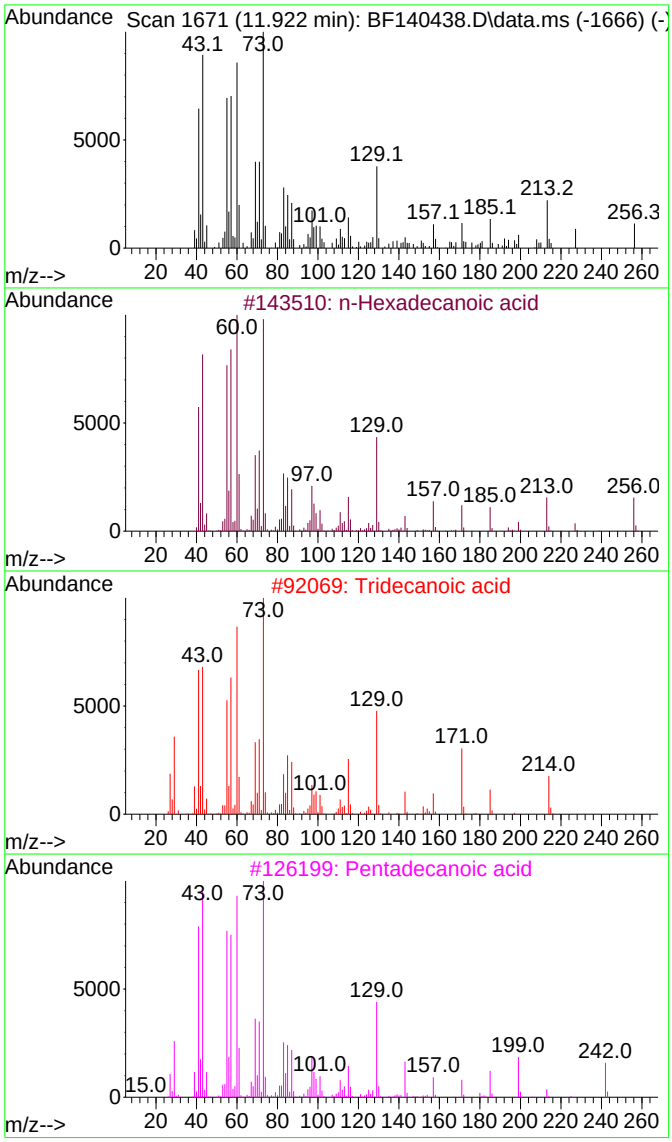
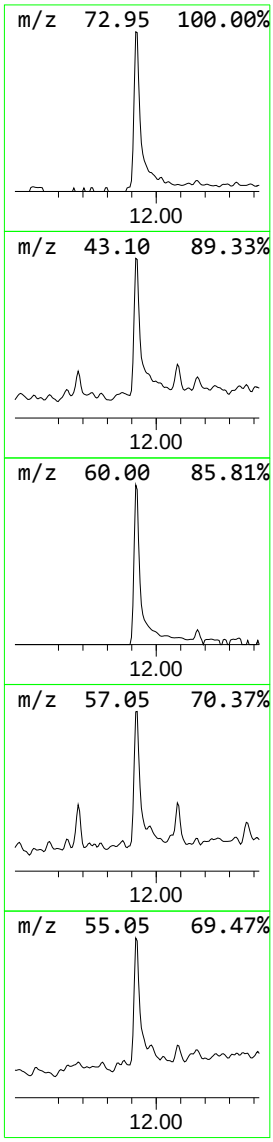
Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.31 ng	146006	Phenanthrene-d10	11.398

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

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TIC Integration Parameters: LSCINT.P

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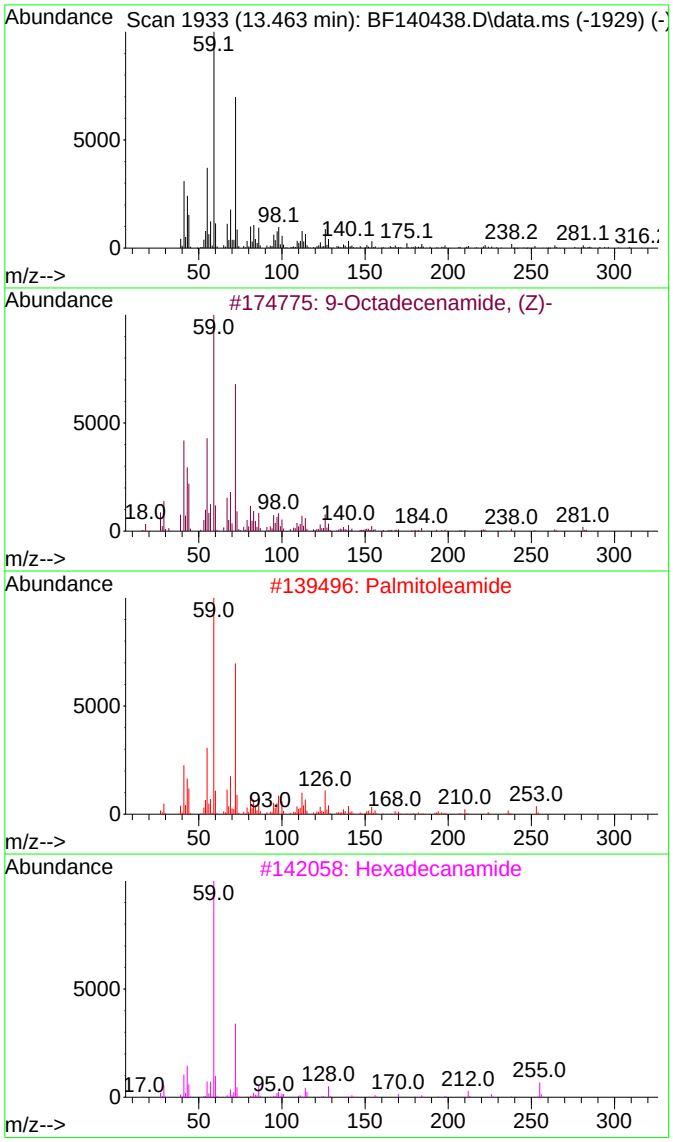
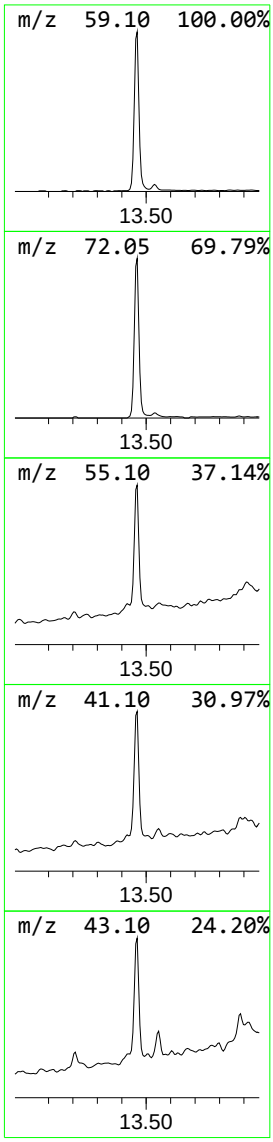
Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	9.21 ng	294038	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Octanamide	143	C8H17NO	000629-01-6	59





Tentatively Identified Compound (LSC) summary

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Data File : BF140438.D
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Sample : P4768-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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
2-Pentanone, 4-...	5.087	3.2	ng	121767	1	6.875	769640	20.0
Cyclohexane, 1,...	5.293	3.1	ng	118922	1	6.875	769640	20.0
Cyclohexane, 1-...	5.693	2.0	ng	77116	1	6.875	769640	20.0
Nonane	5.781	4.5	ng	171567	1	6.875	769640	20.0
Cyclohexane, 1-...	5.898	2.4	ng	92377	1	6.875	769640	20.0
Cyclopentane, (...	6.122	2.5	ng	97552	1	6.875	769640	20.0
Decane	6.704	4.2	ng	159786	1	6.875	769640	20.0
Benzophenone	10.622	6.6	ng	323349	3	9.910	980141	20.0
n-Hexadecanoic ...	11.922	3.3	ng	146006	4	11.398	882469	20.0
9-Octadecenamid...	13.463	9.2	ng	294038	5	14.045	638795	20.0