LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047442.D
Acq On : 04 Sep 2024 17:23
Operator : RC/JU
Sample : P3750-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
72-11978

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_M\Methods\8270-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	60	64	73	rBV	96181	153438	2.12%	0.343%
2	4.557	276	284	296	rVB	152045	229134	3.17%	0.512%
3	5.010	355	361	385	rBV	2492789	3757547	51.96%	8.401%
4	6.575	620	627	653	rBV	2063962	3731956	51.60%	8.344%
5	7.340	750	757	768	rBV	765864	1219956	16.87%	2.728%
6	8.492	946	953	978	rBV	1352628	2447159	33.84%	5.472%
7	10.098	1219	1226	1242	rBV	848180	1518538	21.00%	3.395%
8	10.875	1352	1358	1371	rBV	83979	221684	3.07%	0.496%
9	12.610	1646	1653	1678	rBV	3432311	5717889	79.06%	12.784%
10	14.004	1884	1890	1898	rBV	1218247	1928747	26.67%	4.312%
11	14.069	1898	1901	1912	rVB	41316	86896	1.20%	0.194%
12	14.239	1925	1930	1931	rBV	115889	154208	2.13%	0.345%
13	14.257	1931	1933	1940	rVB	135118	162856	2.25%	0.364%
14	15.527	2142	2149	2173	rBV	2442685	4113585	56.88%	9.197%
15	16.774	2356	2361	2366	rBV	1506170	2178115	30.12%	4.870%
16	16.815	2366	2368	2376	rVB	182226	304474	4.21%	0.681%
17	16.915	2381	2385	2391	rVB	51978	93778	1.30%	0.210%
18	17.709	2515	2520	2529	rBV	876687	1337914	18.50%	2.991%
19	17.845	2539	2543	2548	rBV2	55587	88070	1.22%	0.197%
20	18.856	2710	2715	2727	rBV	517279	891553	12.33%	1.993%
21	19.009	2737	2741	2750	rBV	494206	772665	10.68%	1.728%
22	19.221	2770	2777	2783	rBV	462092	718959	9.94%	1.607%
23	19.439	2809	2814	2826	rVB	5797472	7232249	100.00%	16.170%
24	20.739	3032	3035	3042	rVB3	478401	618368	8.55%	1.383%
25	21.021	3077	3083	3087	rBV2	1787775	2592833	35.85%	5.797%
26	23.727	3537	3543	3551	rVB	1107869	2452836	33.92%	5.484%

Sum of corrected areas: 44725407

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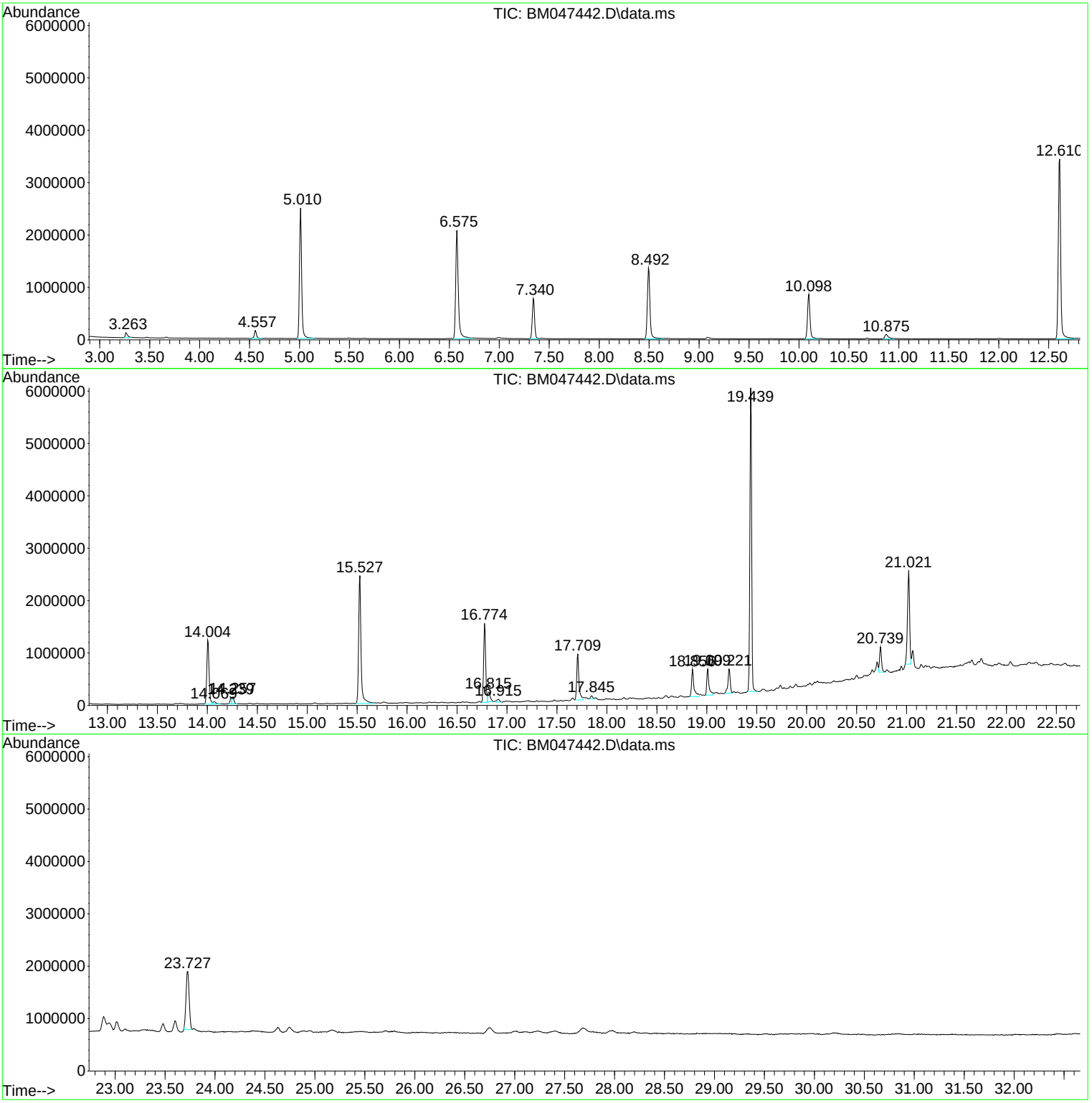
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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TIC Library : C:\Database\NIST20.L
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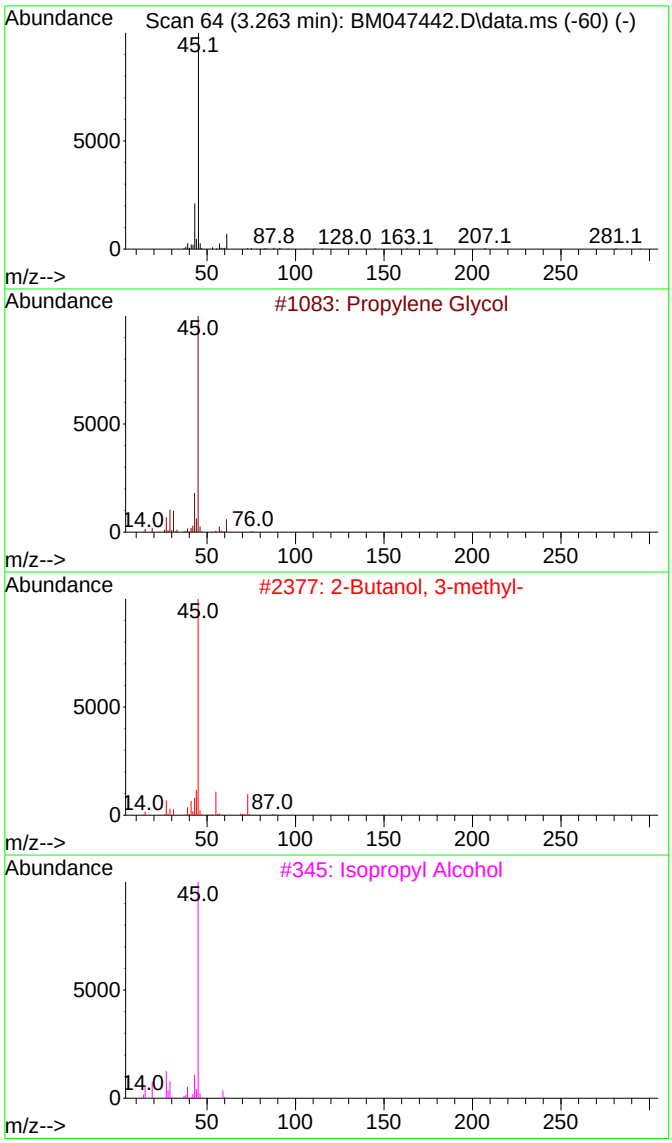
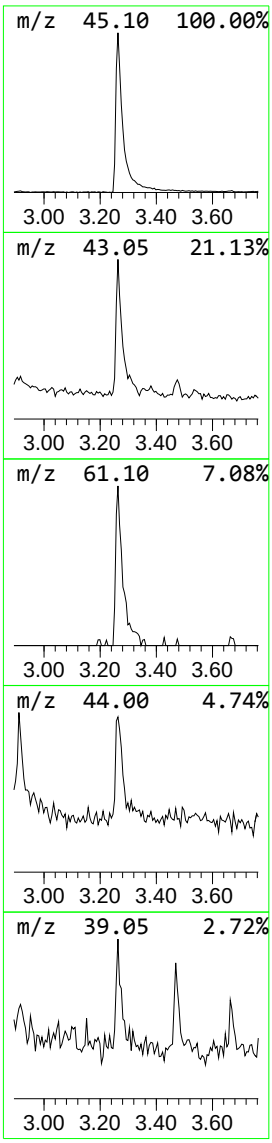
Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.263	2.52 ng	153438	1,4-Dichlorobenzene-d4	7.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	56
2	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
5	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	9





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Sample : P3750-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
72-11978

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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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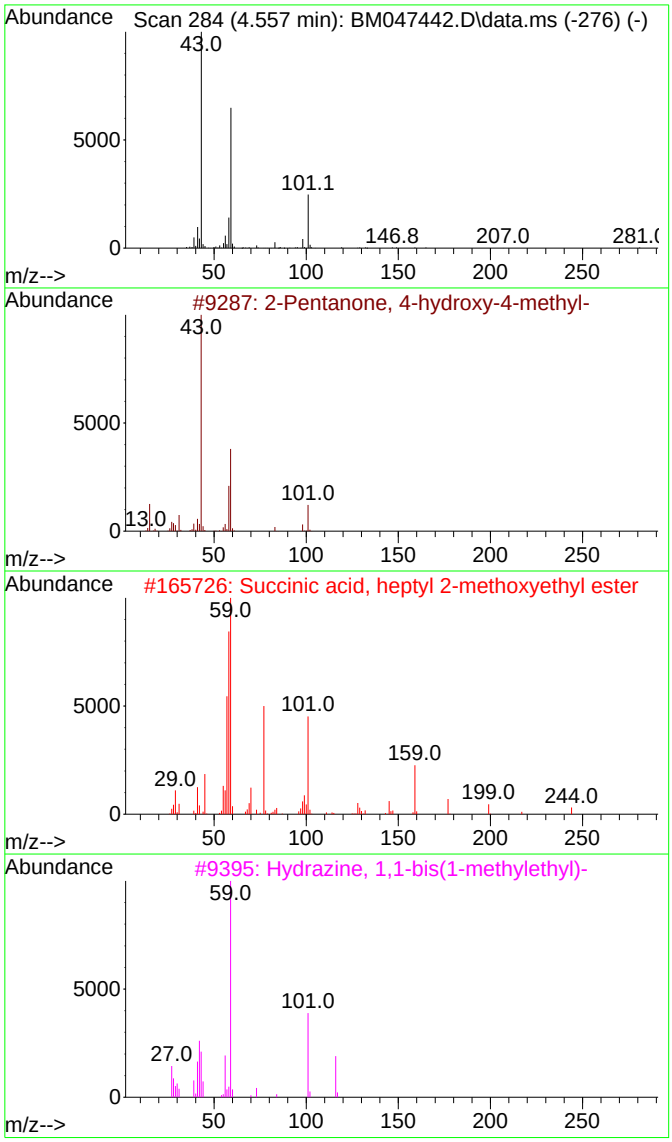
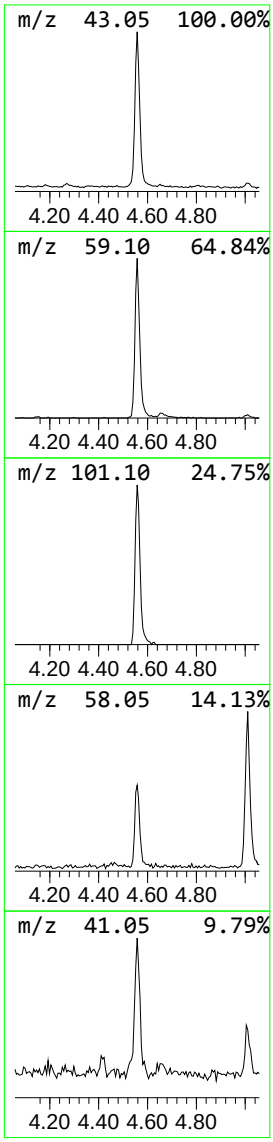
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	3.76 ng	229134	1,4-Dichlorobenzene-d4	7.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	Tetraglyme	222	C10H22O5	000143-24-8	25
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25





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Data File : BM047442.D
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Operator : RC/JU
Sample : P3750-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
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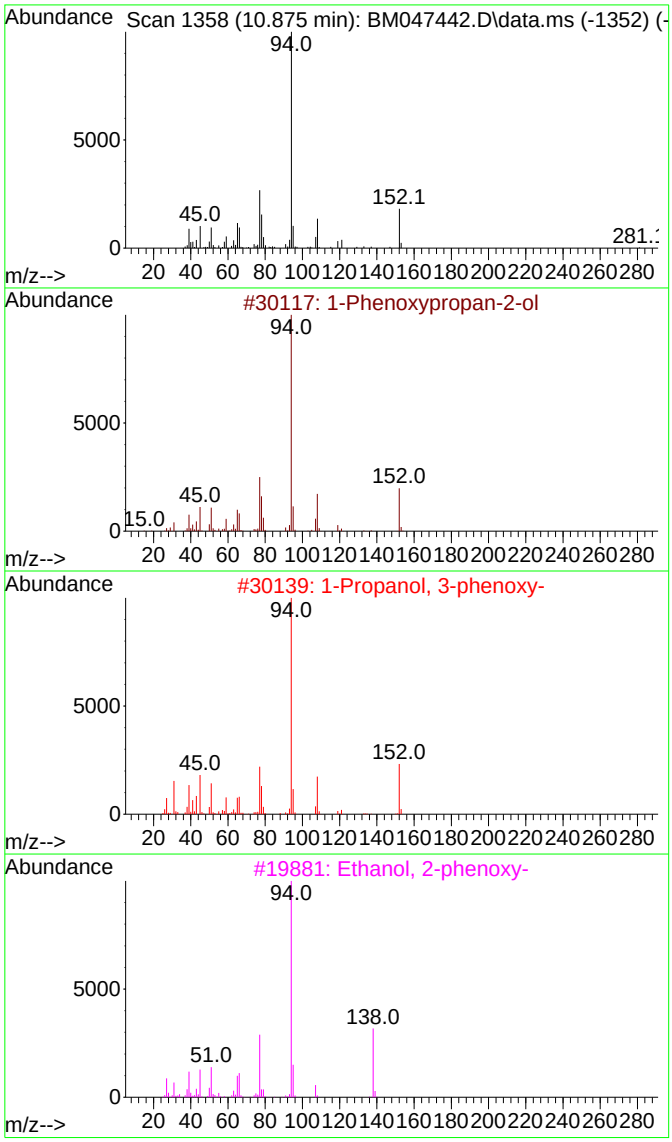
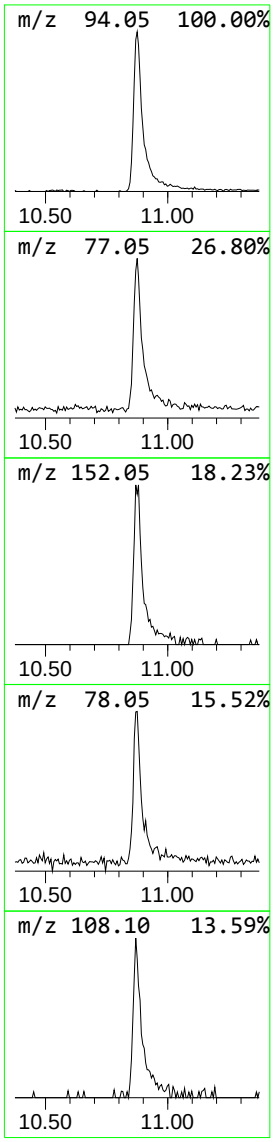
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.92 ng	221684	Naphthalene-d8	10.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	Benzene, (3-bromopropoxy)-	214	C9H11BrO	000588-63-6	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
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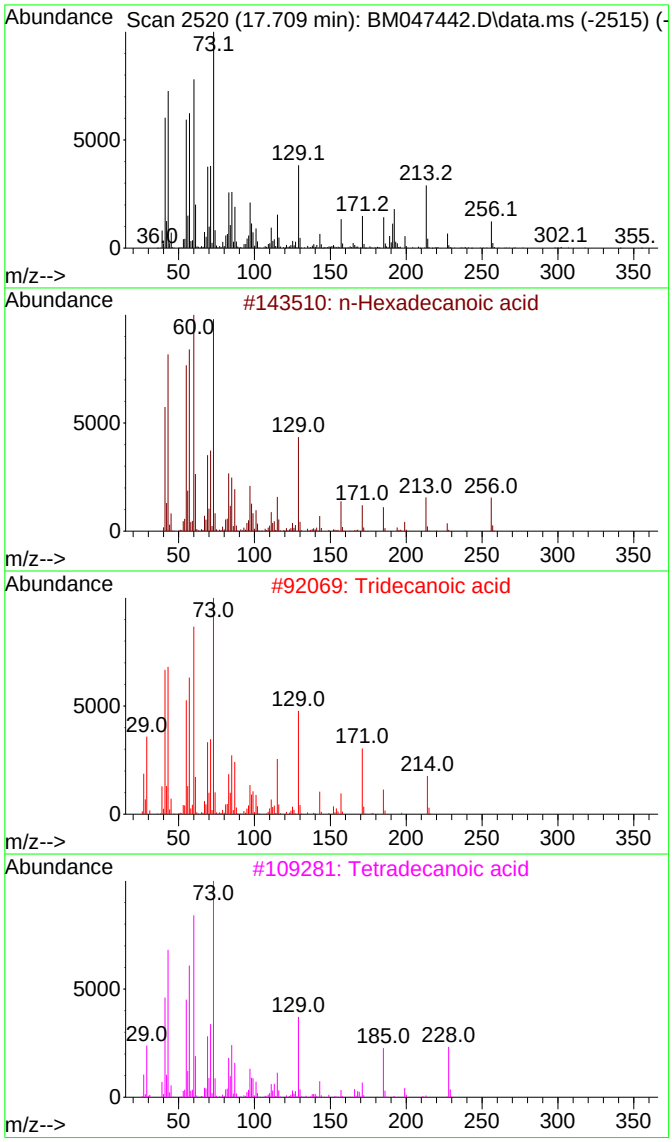
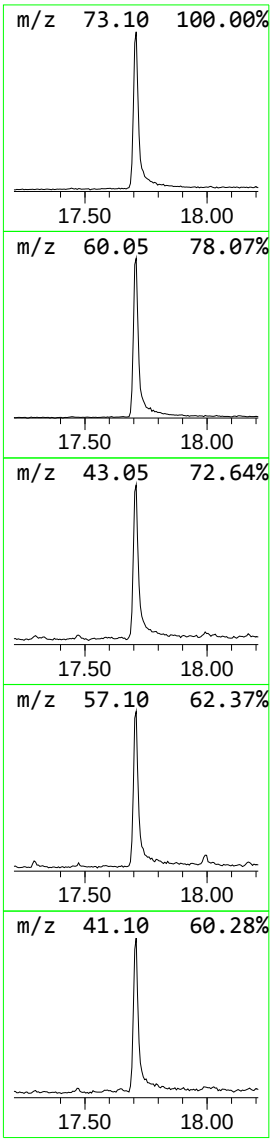
Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	12.29 ng	1337910	Phenanthrene-d10	16.774

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





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Sample : P3750-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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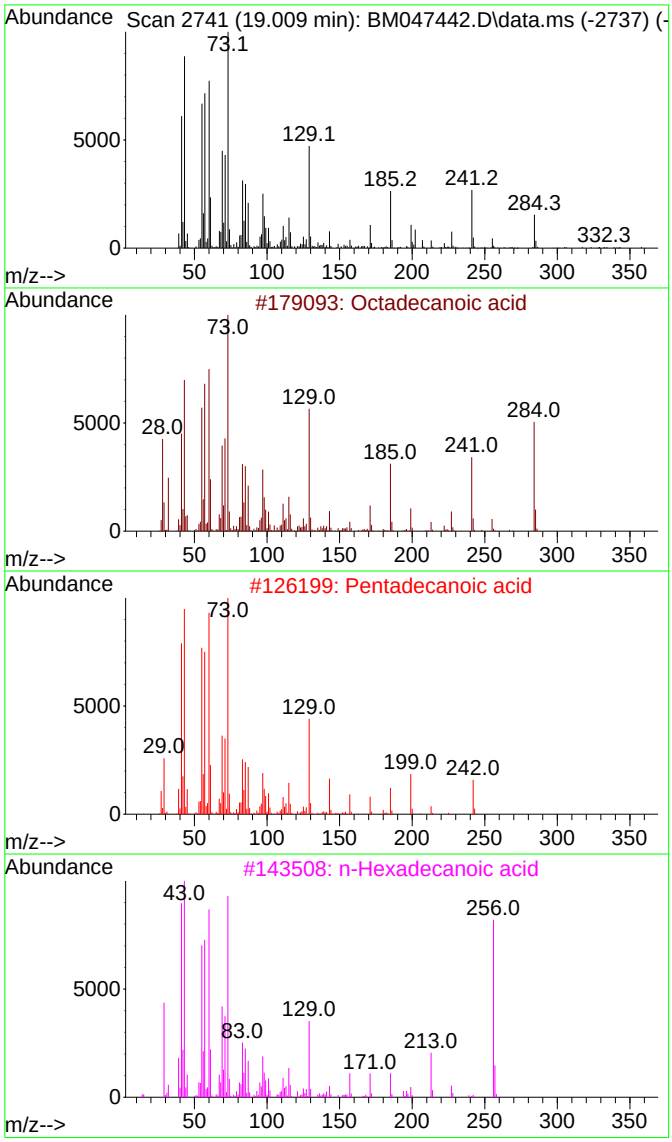
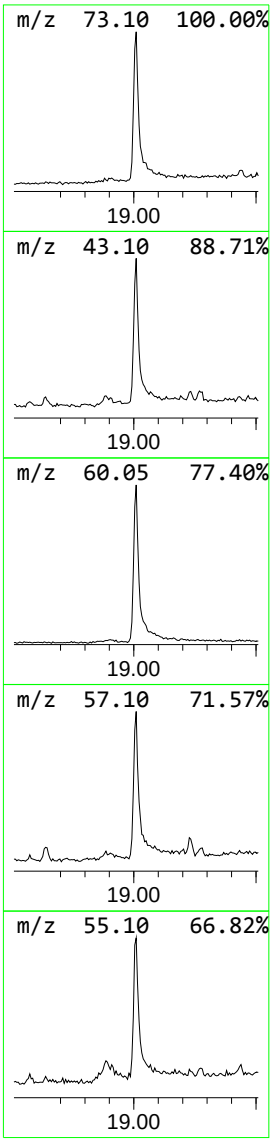
Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	5.96 ng	772665	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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

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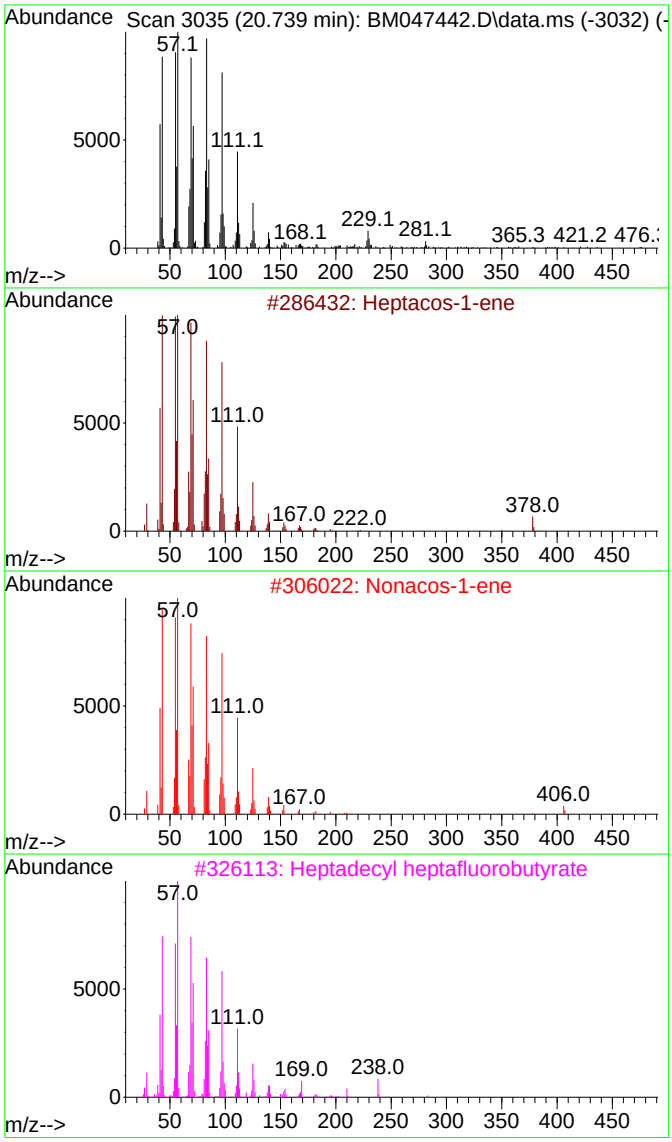
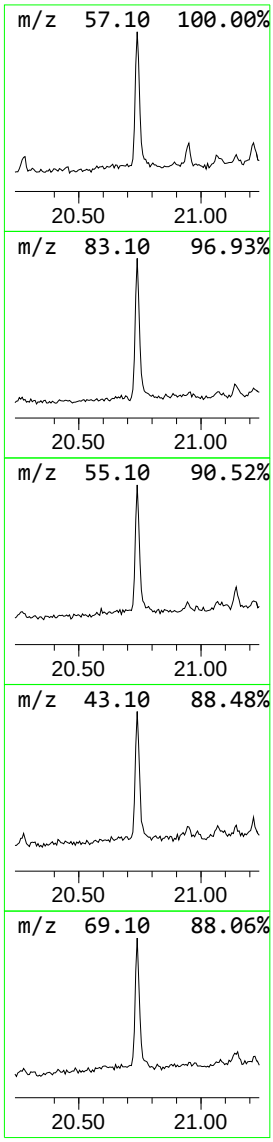
Peak Number 6 Heptacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.739	4.77 ng	618368	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	94
2	Nonacos-1-ene	406	C29H58	018835-35-3	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Tentatively Identified Compound (LSC) summary

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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
Propylene Glycol	3.263	2.5	ng	153438	1	7.340	1219960	20.0
2-Pentanone, 4-...	4.557	3.8	ng	229134	1	7.340	1219960	20.0
1-Phenoxypropan...	10.875	2.9	ng	221684	2	10.098	1518540	20.0
n-Hexadecanoic ...	17.709	12.3	ng	1337910	4	16.774	2178120	20.0
Octadecanoic acid	19.009	6.0	ng	772665	5	21.021	2592830	20.0
Heptacos-1-ene	20.739	4.8	ng	618368	5	21.021	2592830	20.0