LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050145.D
Acq On : 08 May 2025 14:02
Operator : RC/JU
Sample : Q1964-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-LL

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-BM042825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.475	80	83	101	rVB	226335	382502	3.13%	0.503%
2	4.863	311	319	327	rBV	367634	537529	4.40%	0.707%
3	5.334	393	399	419	rBV	3709963	5686900	46.53%	7.476%
4	6.934	661	671	686	rBV	3115328	5689442	46.55%	7.479%
5	7.740	798	808	818	rBV	836777	1342623	10.98%	1.765%
6	8.899	998	1005	1023	rBV	1914222	3608527	29.52%	4.744%
7	10.534	1276	1283	1298	rBV	888516	1680569	13.75%	2.209%
8	11.298	1406	1413	1433	rBV	156177	435545	3.56%	0.573%
9	13.004	1696	1703	1719	rBV	5429682	8150803	66.68%	10.715%
10	14.392	1931	1939	1954	rBV	1453231	2275816	18.62%	2.992%
11	14.616	1968	1977	1984	rBV	511726	1165839	9.54%	1.533%
12	14.828	2005	2013	2024	rBV3	160793	381670	3.12%	0.502%
13	15.886	2187	2193	2209	rBV	4692471	7171146	58.67%	9.427%
14	16.551	2302	2306	2319	rBV7	62211	165705	1.36%	0.218%
15	17.139	2400	2406	2421	rBV2	1722704	2639140	21.59%	3.469%
16	17.527	2467	2472	2482	rVB	140666	236874	1.94%	0.311%
17	17.810	2516	2520	2530	rVB4	93593	207773	1.70%	0.273%
18	18.045	2553	2560	2584	rBV	4770233	7641543	62.52%	10.045%
19	18.457	2626	2630	2635	rVB	180980	210554	1.72%	0.277%
20	19.039	2723	2729	2737	rVB2	129091	258485	2.11%	0.340%
21	19.174	2748	2752	2753	rBV	107229	126980	1.04%	0.167%
22	19.198	2753	2756	2766	rVB4	139150	309039	2.53%	0.406%
23	19.321	2771	2777	2803	rVV	3565634	5803165	47.48%	7.629%
24	19.762	2847	2852	2864	rVB	10221105	12223272	100.00%	16.068%
25	19.939	2877	2882	2894	rVB	216638	357798	2.93%	0.470%
26	20.698	3006	3011	3019	rBV	308457	448989	3.67%	0.590%
27	21.057	3068	3072	3081	rBV	403829	623483	5.10%	0.820%
28	21.386	3122	3128	3132	rBV	1978795	2996308	24.51%	3.939%
29	24.374	3629	3636	3652	rVB	1247553	3312471	27.10%	4.354%

Sum of corrected areas: 76070490

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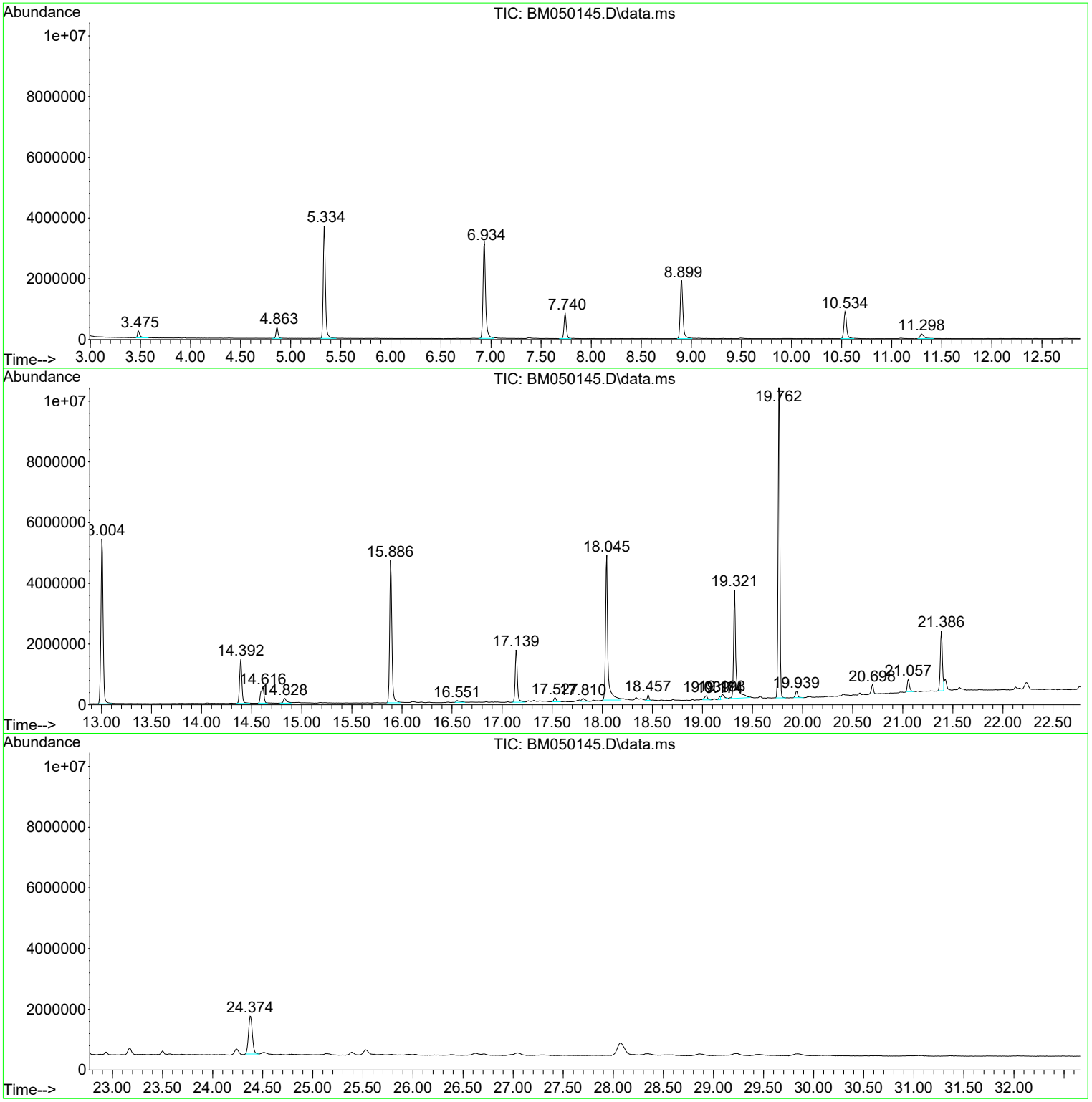
Instrument :
BNA_M
ClientSampleId :
MH-LL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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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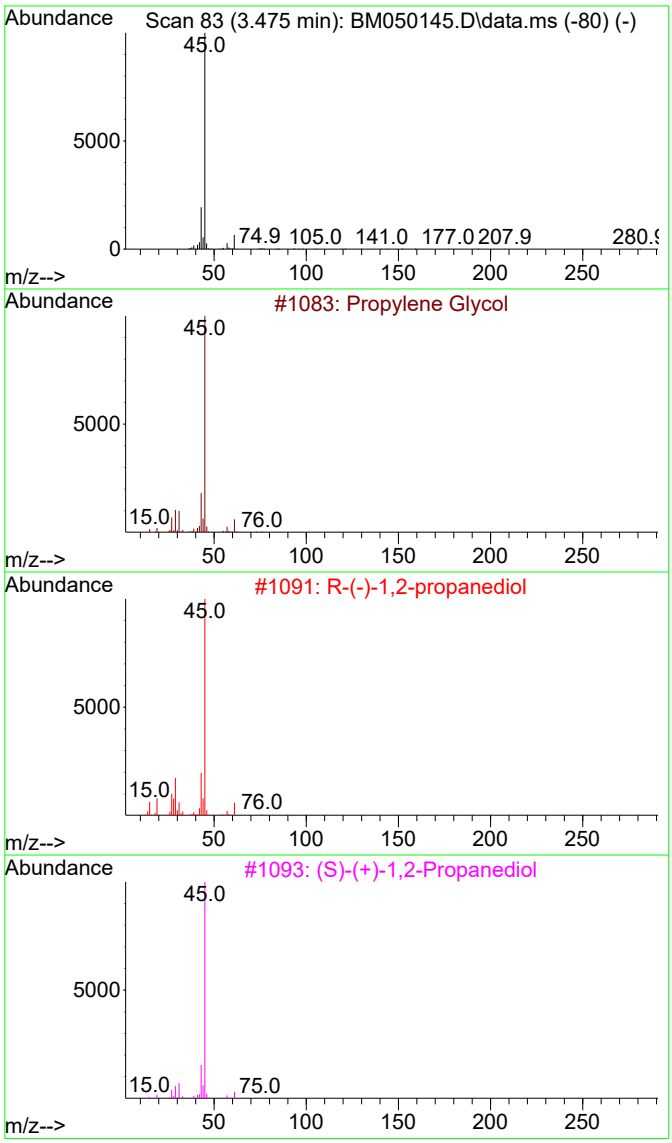
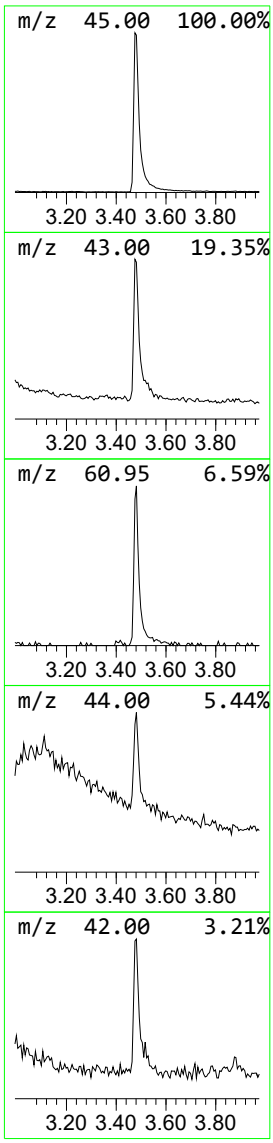
Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.475	5.70 ng	382502	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





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Acq On : 08 May 2025 14:02
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Sample : Q1964-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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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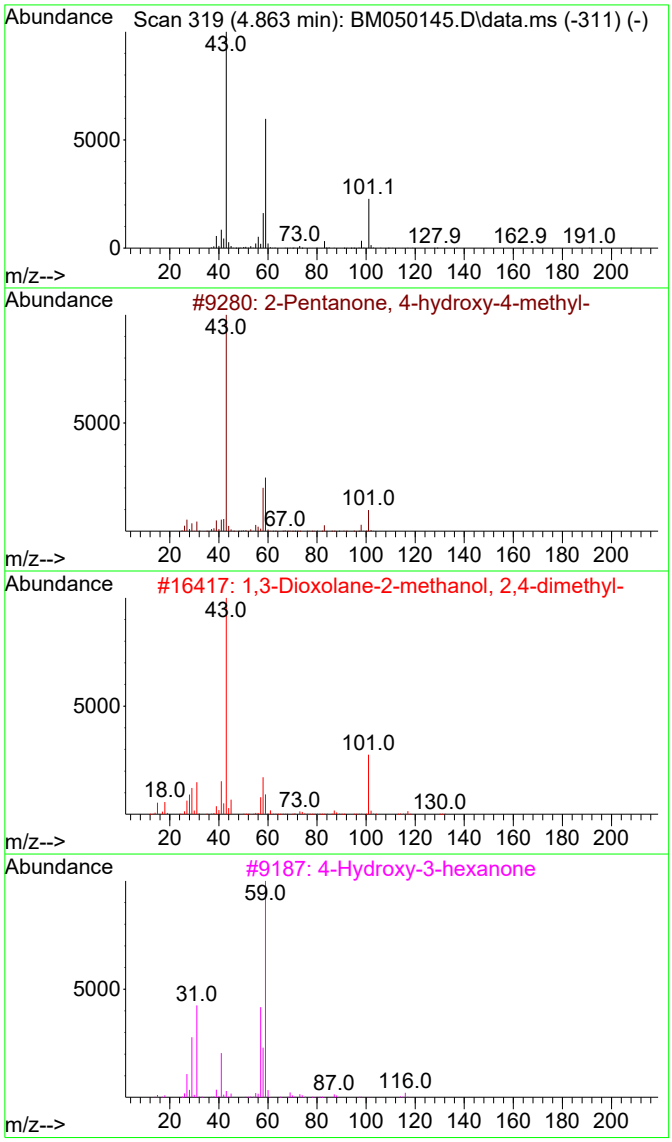
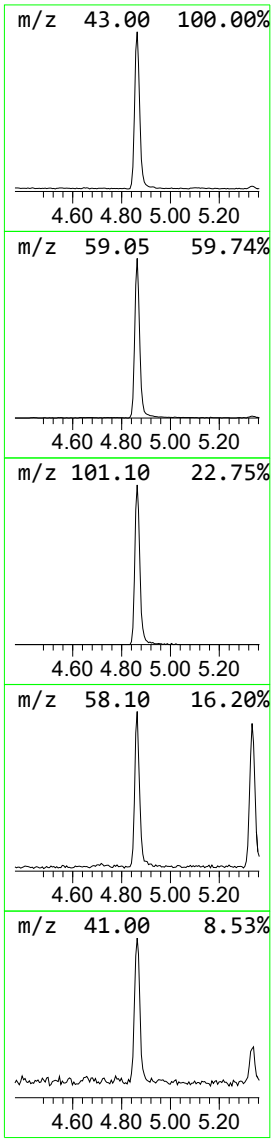
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	8.01 ng	537529	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument :
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ClientSampleId :
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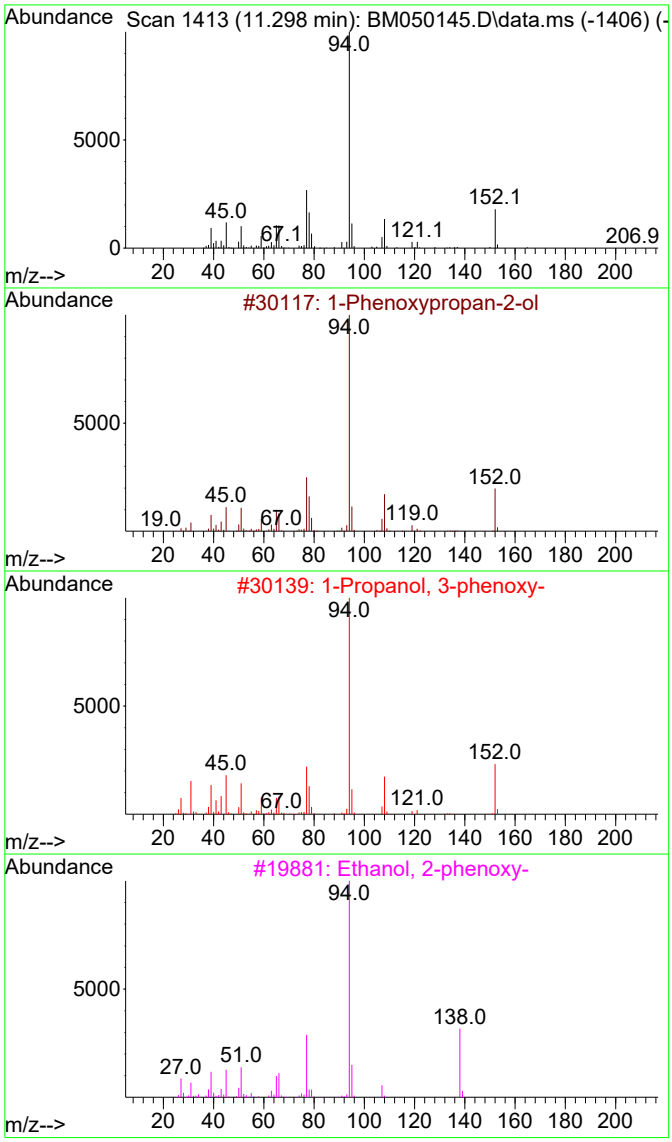
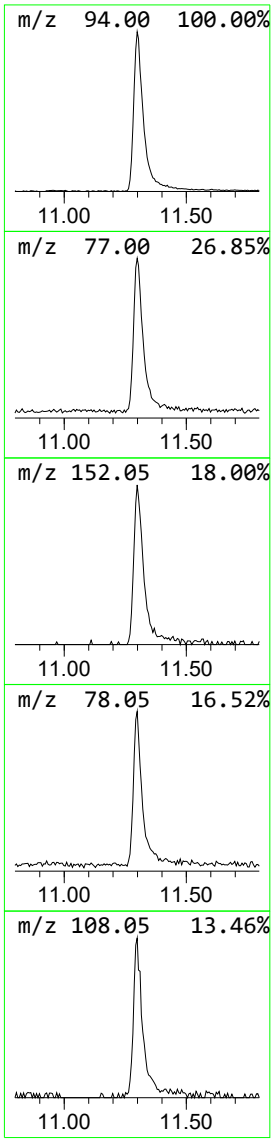
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	5.18 ng	435545	Naphthalene-d8	10.534

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	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
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TIC Library : C:\Database\NIST20.L
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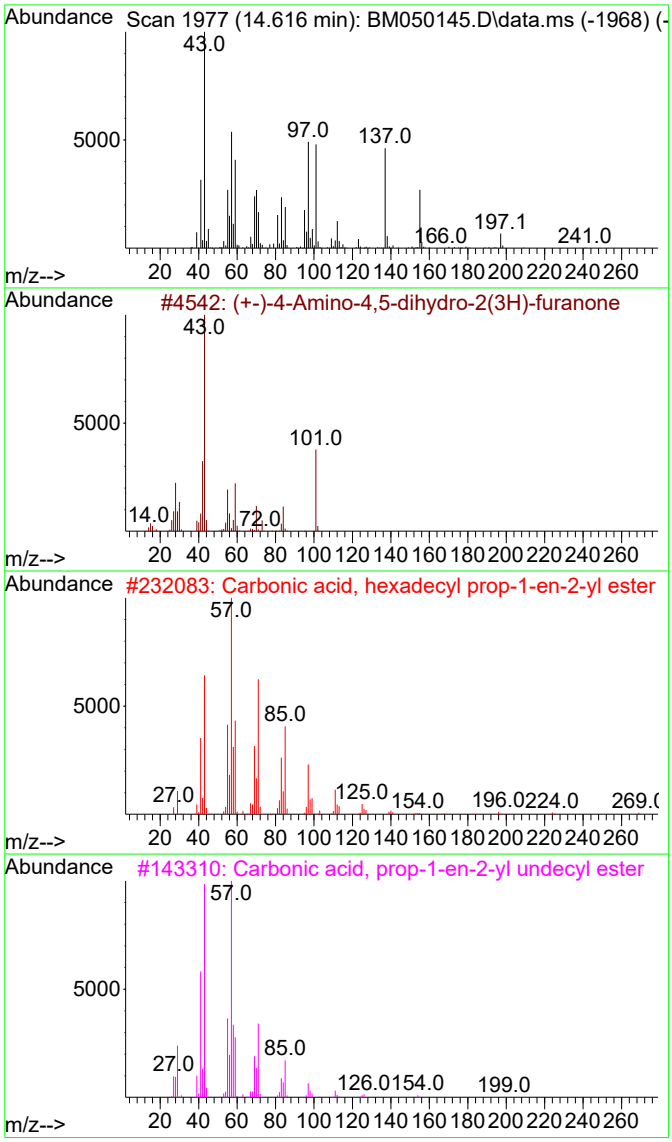
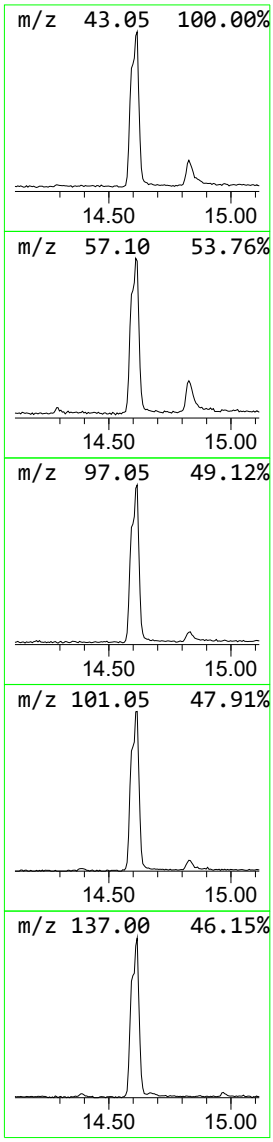
Peak Number 4 unknown14.616 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	10.25 ng	1165840	Acenaphthene-d10	14.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	30
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	16
3	Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
4	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
5	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10





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Sample : Q1964-01
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Instrument :
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ClientSampleId :
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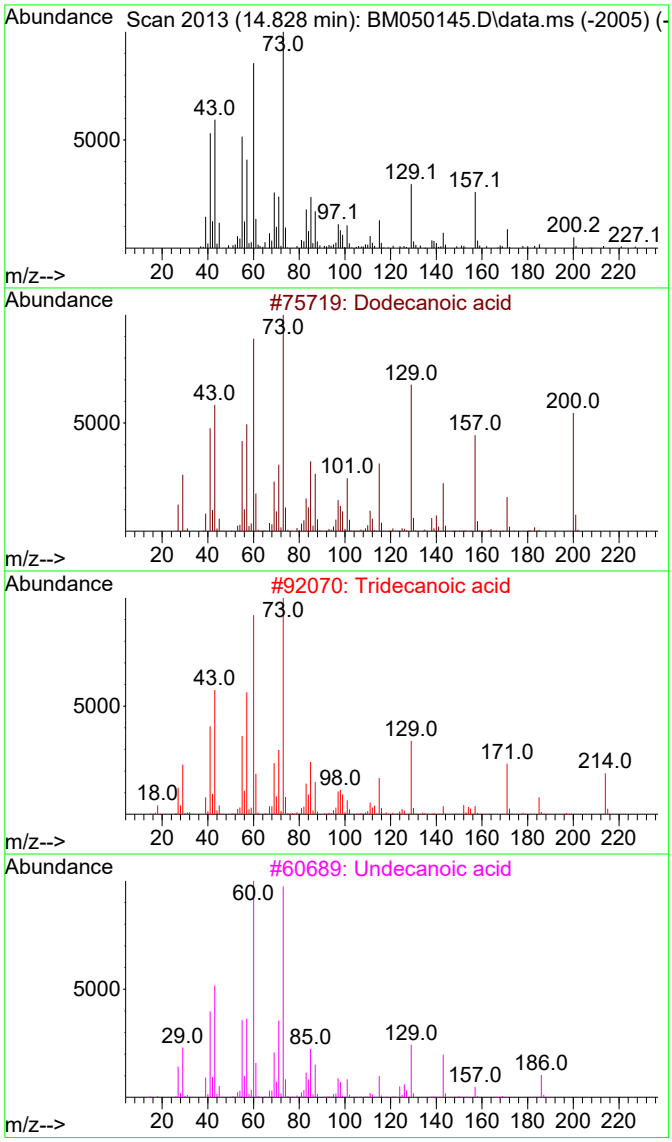
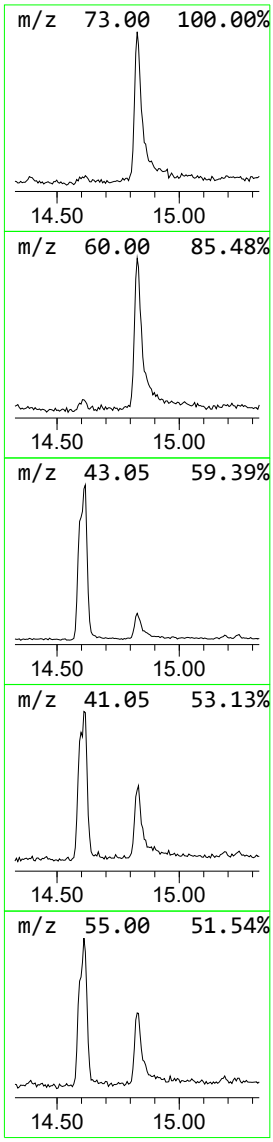
Peak Number 5 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.828	3.35 ng	381670	Acenaphthene-d10	14.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	49





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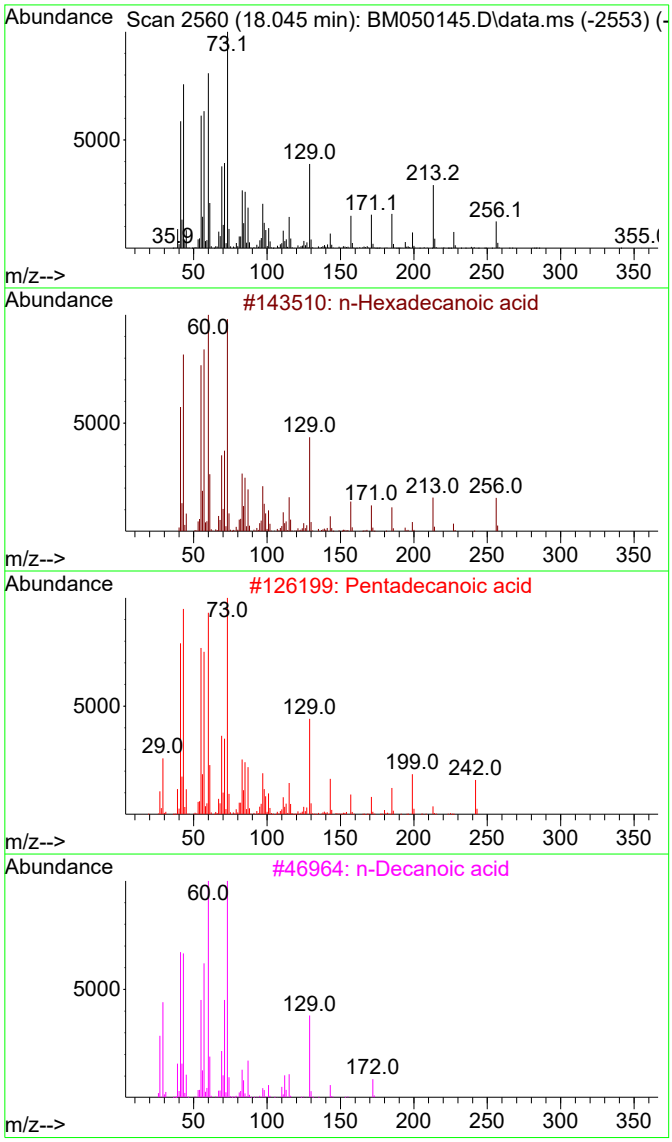
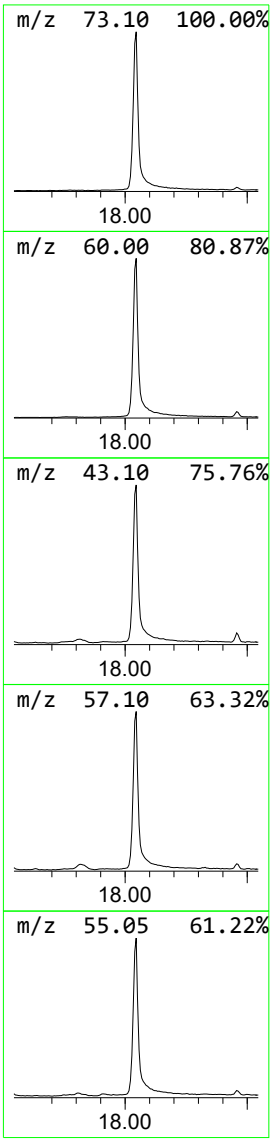
Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	57.91 ng	7641540	Phenanthrene-d10	17.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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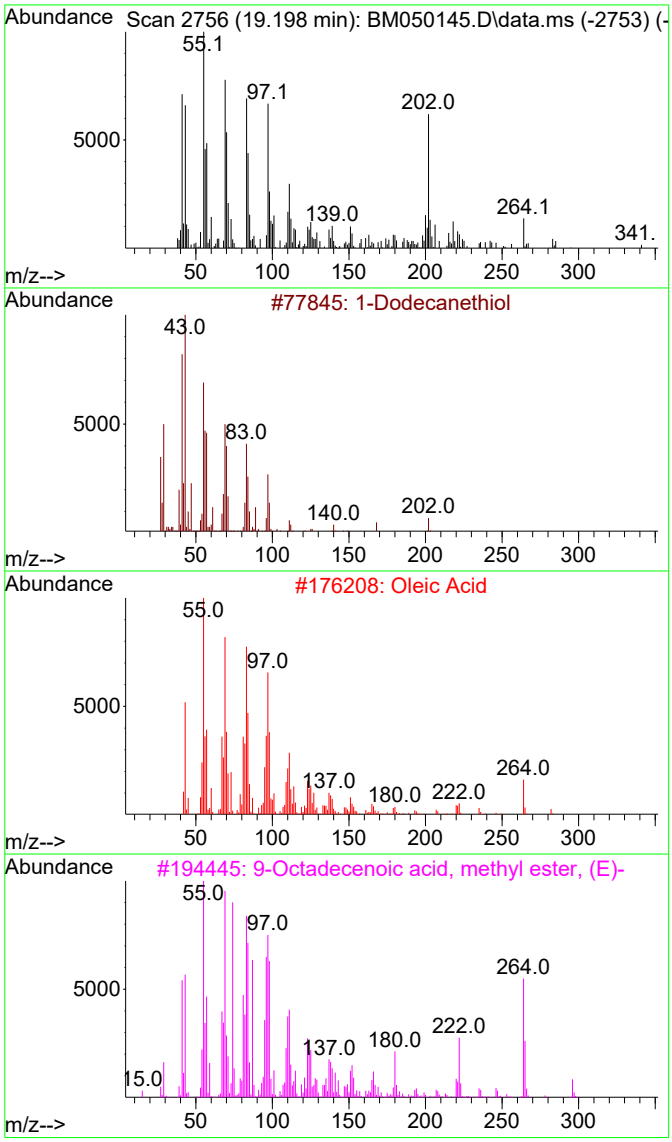
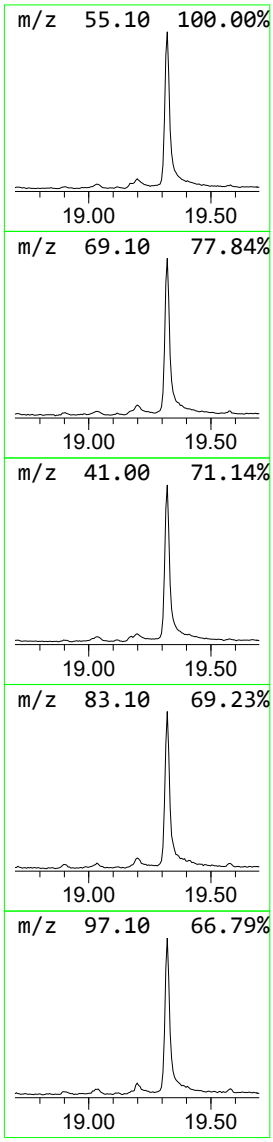
Peak Number 7 1-Dodecanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.198	2.34 ng	309039	Phenanthrene-d10	17.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanethiol	202	C12H26S	000112-55-0	90
2	Oleic Acid	282	C18H34O2	000112-80-1	81
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	76
4	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	72
5	3-Bromobenzoic acid, tetradecyl ...	396	C21H33BrO2	1000281-95-0	64





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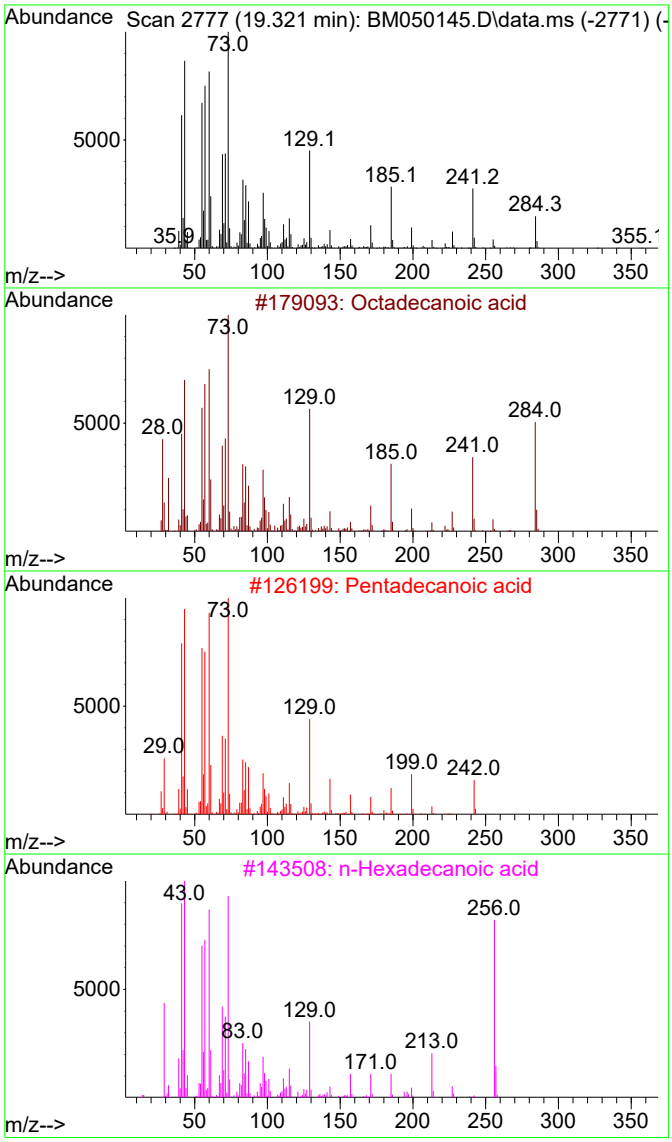
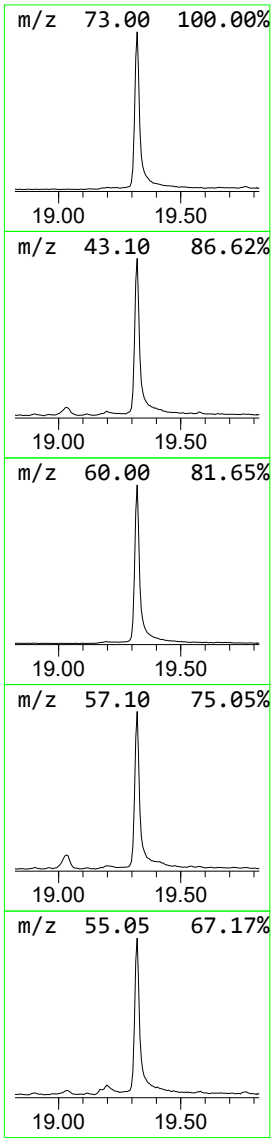
Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	38.74 ng	5803170	Chrysene-d12	21.386

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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TIC Library : C:\Database\NIST20.L
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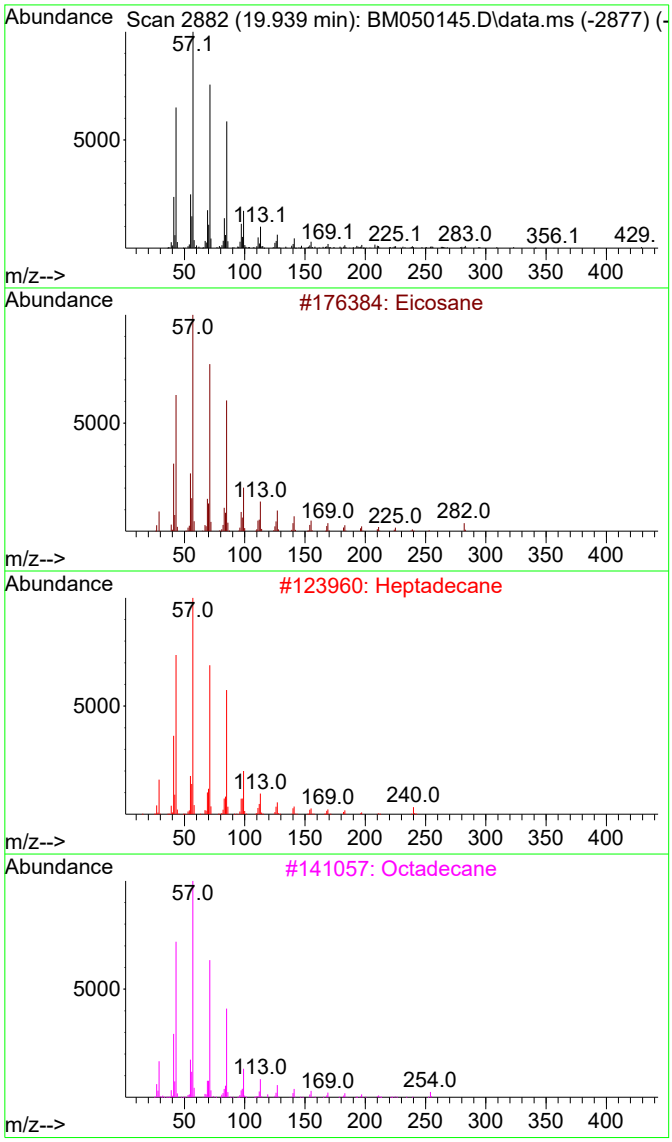
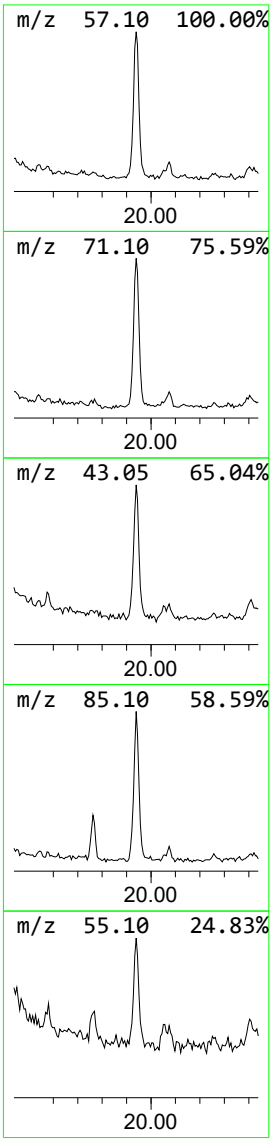
Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.939	2.39 ng	357798	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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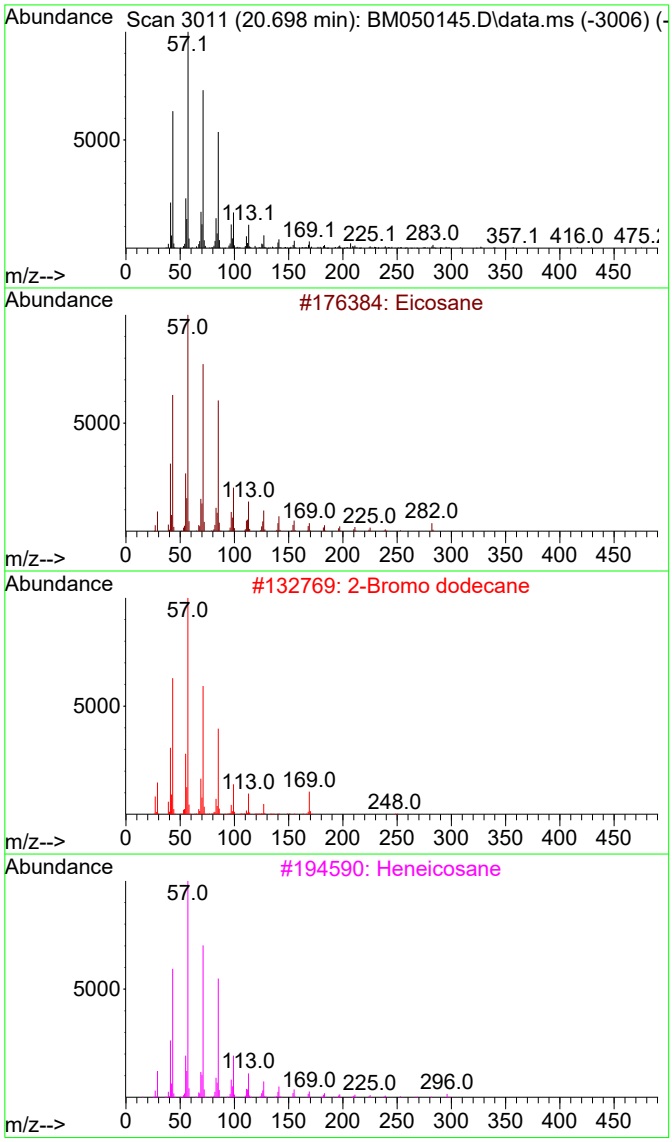
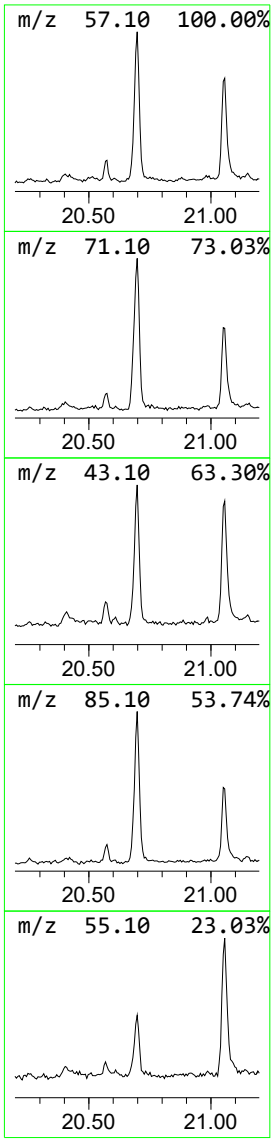
Peak Number 10 2-Bromo dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.698	3.00 ng	448989	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050145.D
Acq On : 08 May 2025 14:02
Operator : RC/JU
Sample : Q1964-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-LL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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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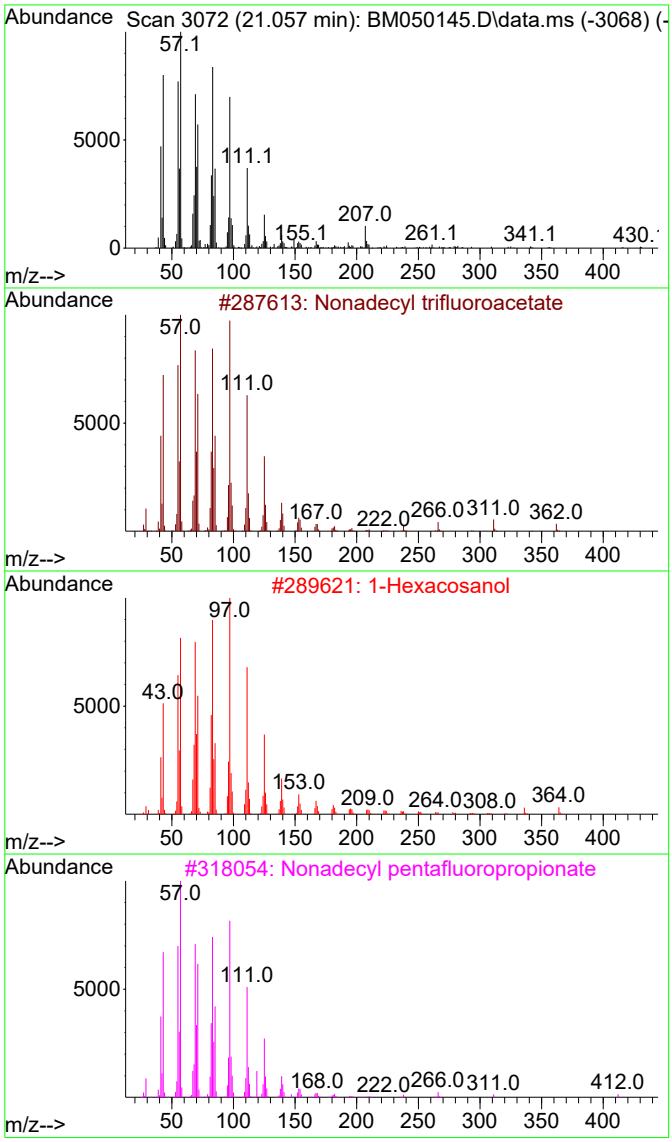
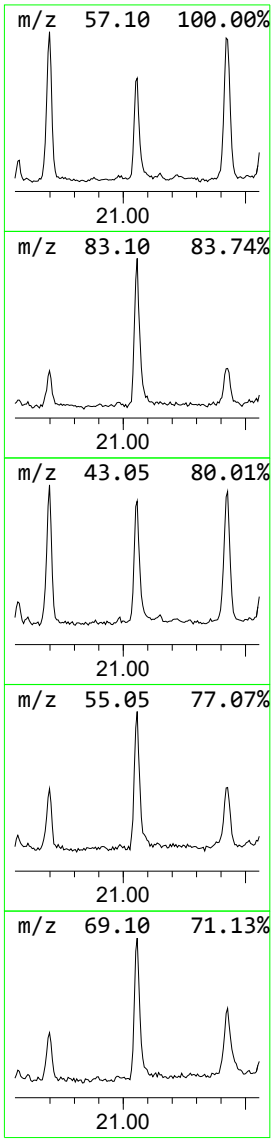
Peak Number 11 Nonadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	4.16 ng	623483	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Octacosanol	410	C28H58O	000557-61-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050145.D
Acq On : 08 May 2025 14:02
Operator : RC/JU
Sample : Q1964-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-LL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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
Propylene Glycol	3.475	5.7	ng	382502	1	7.740	1342620	20.0
2-Pentanone, 4-...	4.863	8.0	ng	537529	1	7.740	1342620	20.0
1-Phenoxypropan...	11.298	5.2	ng	435545	2	10.534	1680570	20.0
unknown14.616	14.616	10.3	ng	1165840	3	14.392	2275820	20.0
Dodecanoic acid	14.828	3.4	ng	381670	3	14.392	2275820	20.0
n-Hexadecanoic ...	18.045	57.9	ng	7641540	4	17.139	2639140	20.0
1-Dodecanethiol	19.198	2.3	ng	309039	4	17.139	2639140	20.0
Octadecanoic acid	19.321	38.7	ng	5803170	5	21.386	2996310	20.0
Eicosane	19.939	2.4	ng	357798	5	21.386	2996310	20.0
2-Bromo dodecane	20.698	3.0	ng	448989	5	21.386	2996310	20.0
Nonadecyl trifl...	21.057	4.2	ng	623483	5	21.386	2996310	20.0