LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050153.D
Acq On : 08 May 2025 19:17
Operator : RC/JU
Sample : Q1972-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WC-B-1

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: BM050153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.487	81	85	99	rBV	113507	198497	2.41%	0.324%
2	4.863	314	319	330	rBV	230715	363398	4.41%	0.594%
3	5.340	393	400	416	rBV	2360121	3886016	47.12%	6.350%
4	6.934	664	671	698	rBV	2013676	4010752	48.63%	6.554%
5	7.740	801	808	822	rBV	938735	1551925	18.82%	2.536%
6	8.904	998	1006	1025	rBV	1166167	2389189	28.97%	3.904%
7	10.533	1275	1283	1302	rBV	993330	2029731	24.61%	3.317%
8	11.310	1408	1415	1429	rBV	64478	213789	2.59%	0.349%
9	13.004	1696	1703	1728	rBV	3491570	5756628	69.80%	9.406%
10	14.392	1931	1939	1948	rBV	1729026	2778617	33.69%	4.540%
11	14.610	1969	1976	1988	rVB2	88542	215141	2.61%	0.352%
12	15.757	2165	2171	2176	rBV	71533	118732	1.44%	0.194%
13	15.892	2186	2194	2214	rBV	3046418	5194076	62.98%	8.487%
14	16.898	2361	2365	2368	rBV	66767	84117	1.02%	0.137%
15	16.945	2370	2373	2384	rVB5	43674	98842	1.20%	0.162%
16	17.139	2400	2406	2411	rBV2	2122349	3257916	39.50%	5.323%
17	17.180	2411	2413	2425	rVB	224163	366107	4.44%	0.598%
18	18.039	2552	2559	2573	rBV2	667435	1328945	16.11%	2.171%
19	18.327	2604	2608	2613	rBV2	78684	113166	1.37%	0.185%
20	19.204	2752	2757	2763	rVB	581521	817275	9.91%	1.335%
21	19.315	2772	2776	2786	rBV2	264103	518982	6.29%	0.848%
22	19.568	2811	2819	2827	rVB	524685	937199	11.36%	1.531%
23	19.762	2847	2852	2858	rVB	7191835	8247072	100.00%	13.476%
24	20.074	2902	2905	2909	rVB2	172591	207381	2.51%	0.339%
25	20.568	2987	2989	2993	rBV	106980	109178	1.32%	0.178%
26	21.050	3067	3071	3083	rVB3	529030	893064	10.83%	1.459%
27	21.380	3121	3127	3132	rBV	2668778	4045951	49.06%	6.611%
28	22.127	3250	3254	3268	rVB	493146	903596	10.96%	1.476%
29	23.080	3412	3416	3424	rVB2	419874	757272	9.18%	1.237%
30	23.497	3482	3487	3493	rVB2	1215118	2248139	27.26%	3.673%
31	23.568	3494	3499	3511	rVB	585454	1489055	18.06%	2.433%
32	24.368	3628	3635	3644	rBV	1399297	3483348	42.24%	5.692%
33	24.838	3708	3715	3726	rVB	1035673	2586586	31.36%	4.226%

Sum of corrected areas: 61199682

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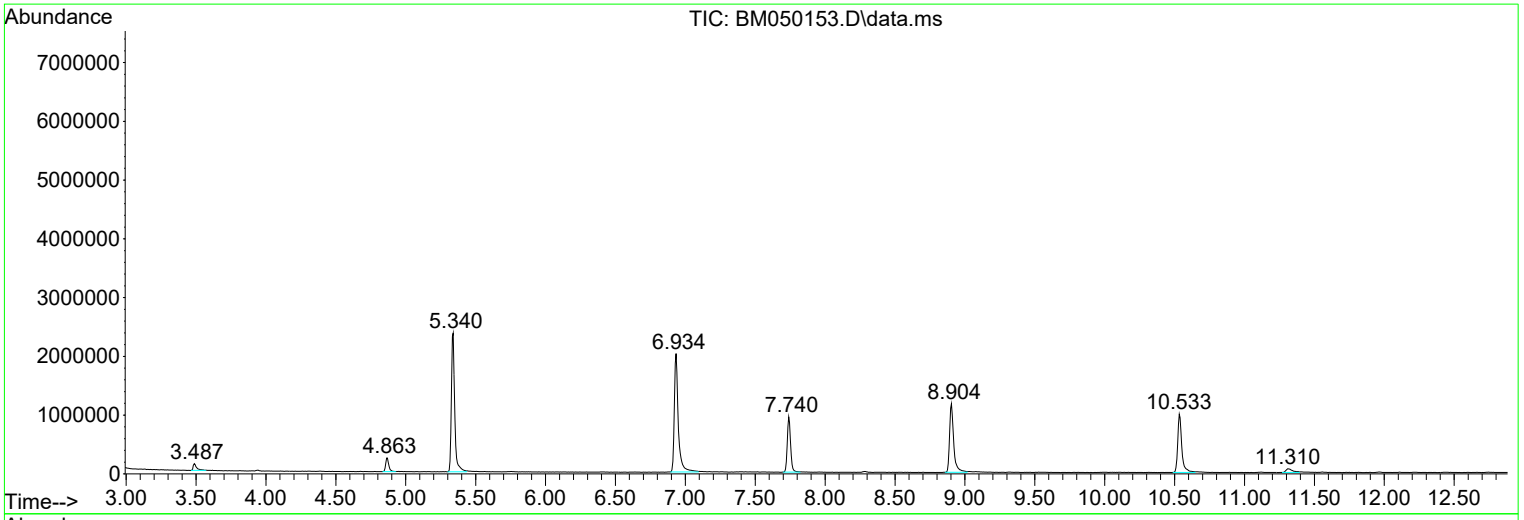
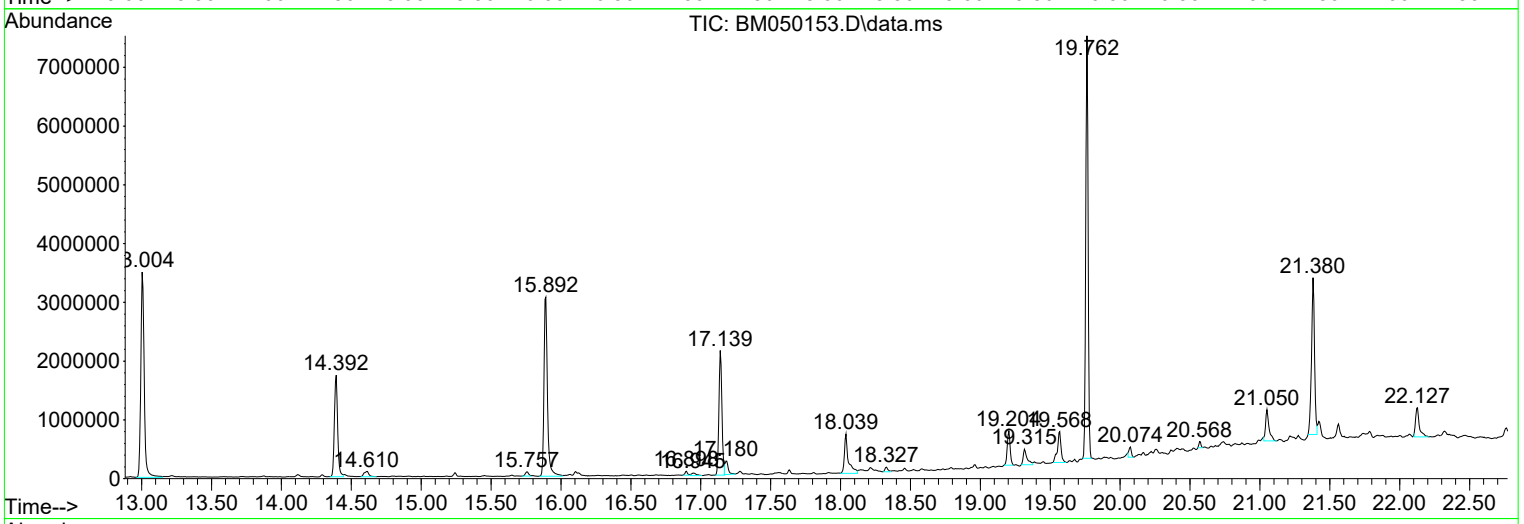
Misc :
ALS Vial : 15 Sample Multiplier: 1

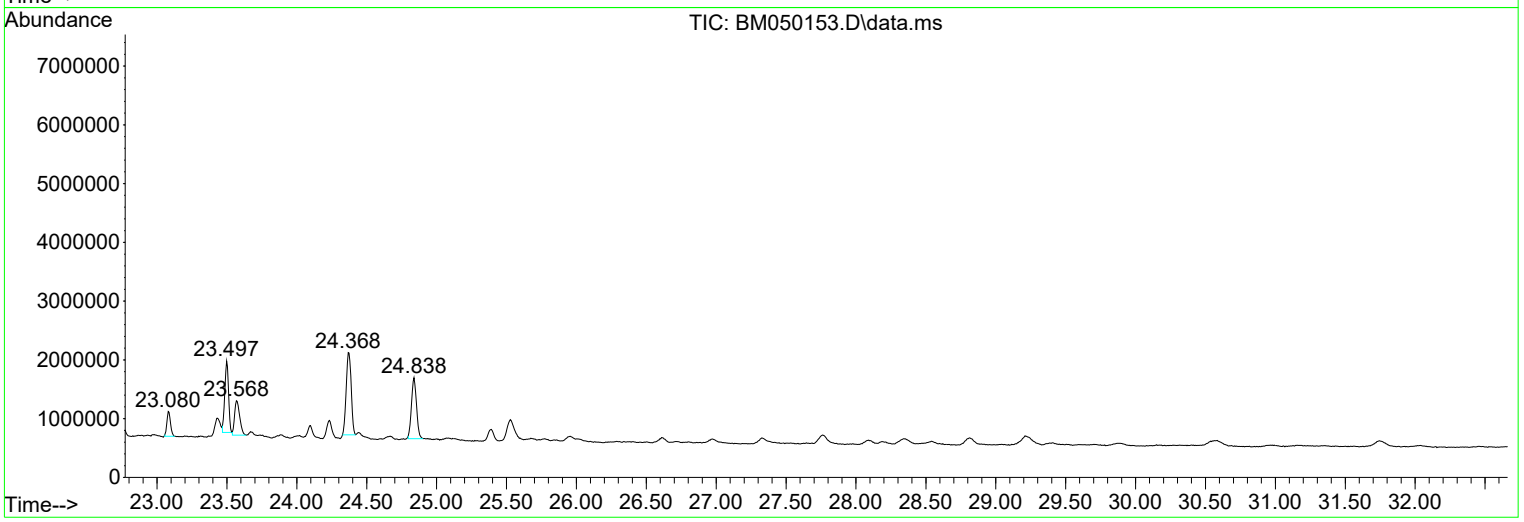
Instrument :
BNA_M
ClientSampleId :
WC-B-1

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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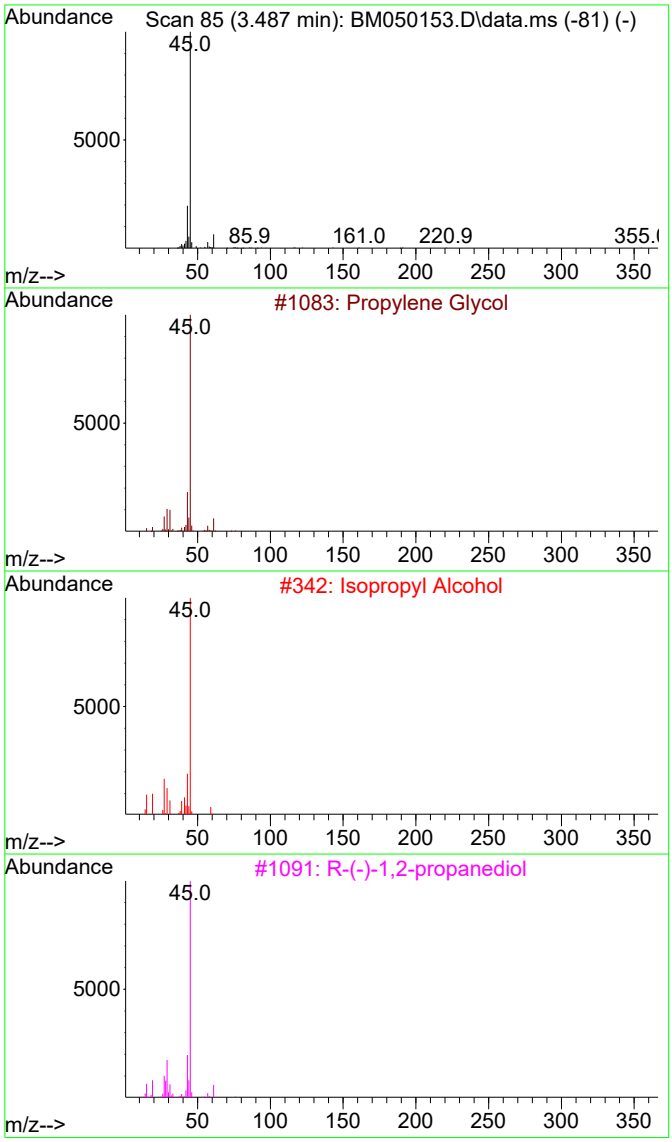
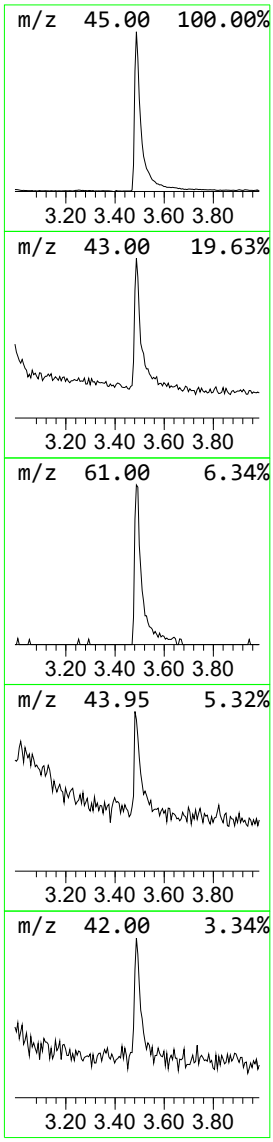
Peak Number 1 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.487	2.56 ng	198497	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	64
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	25
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





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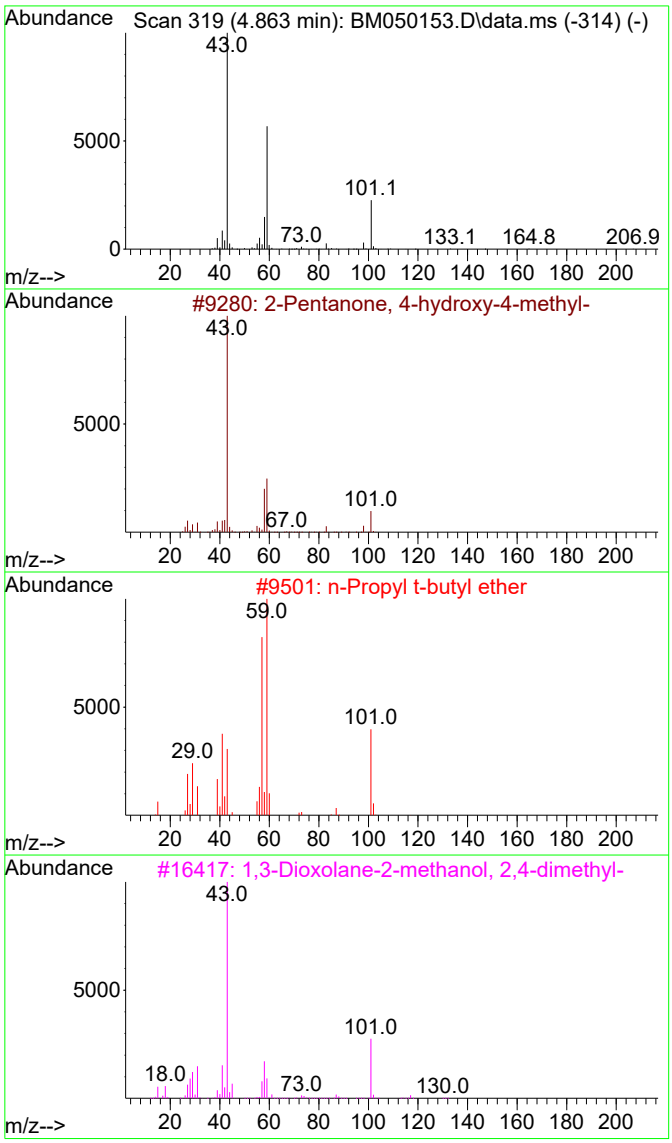
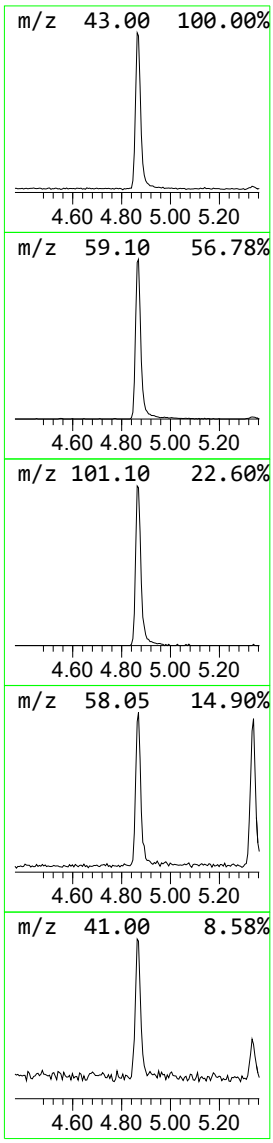
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	4.68 ng	363398	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	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
4	Tetraglyme	222	C10H22O5	000143-24-8	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Misc :
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
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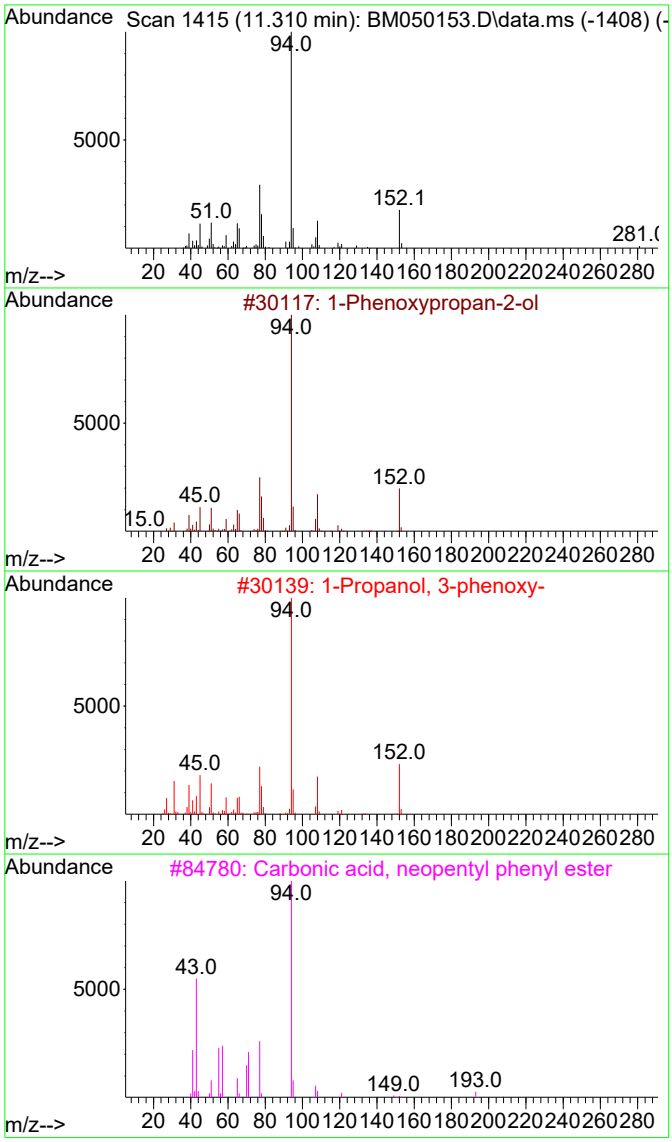
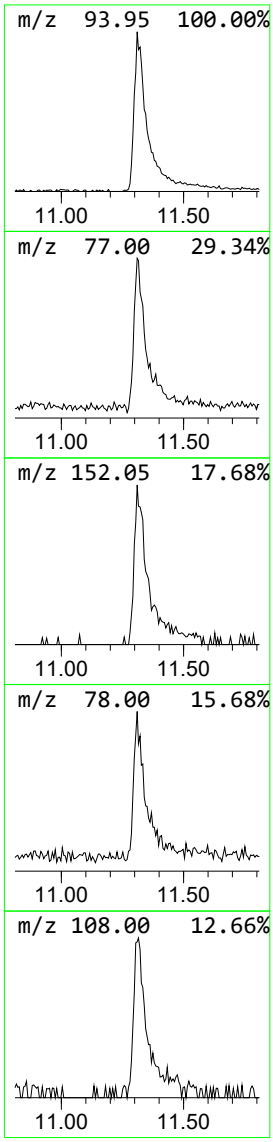
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.310	2.11 ng	213789	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
4	Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53
5	3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	53





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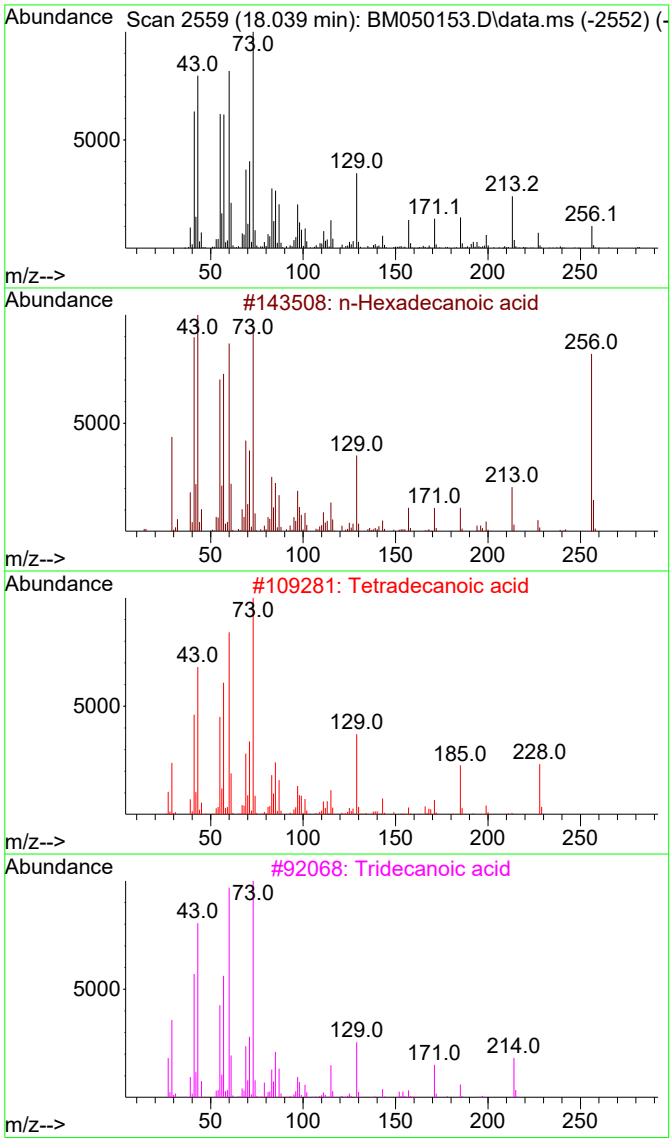
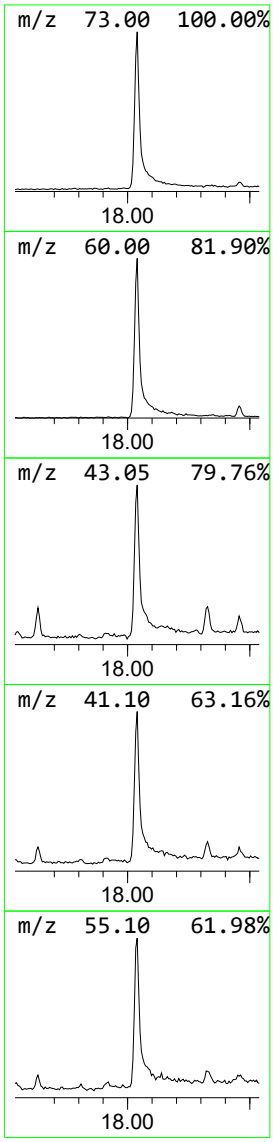
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	8.16 ng	1328950	Phenanthrene-d10	17.139

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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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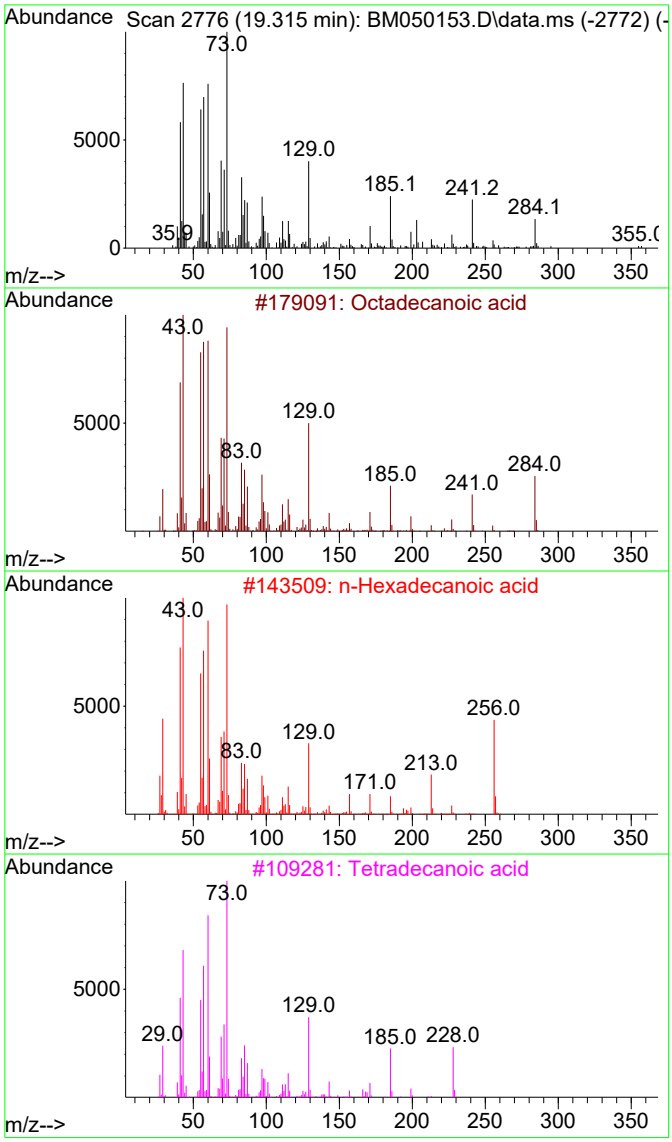
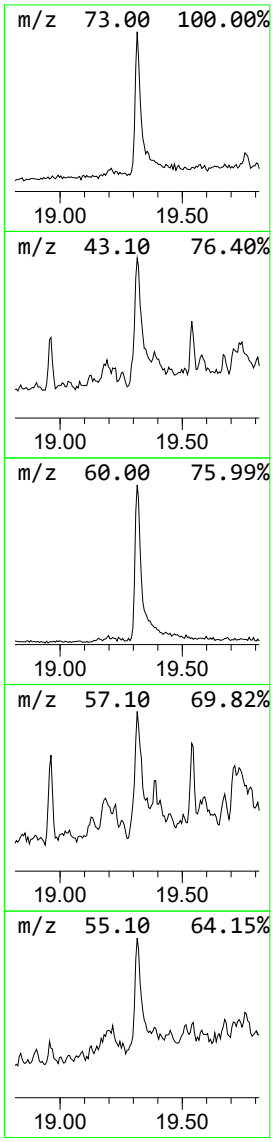
Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.315	2.57 ng	518982	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





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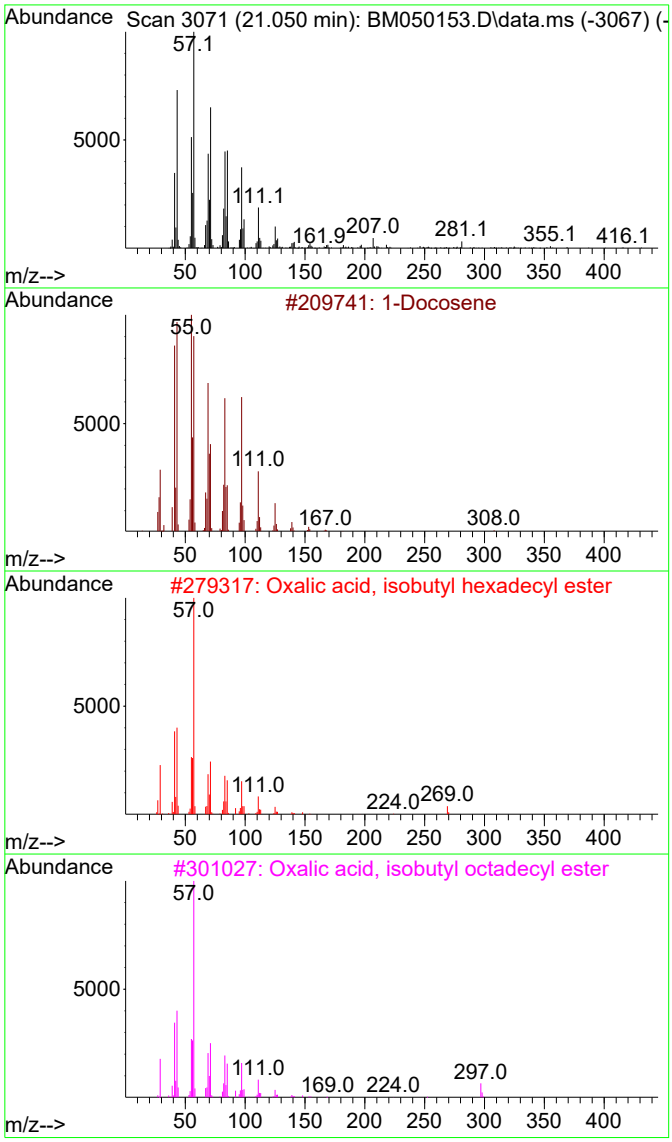
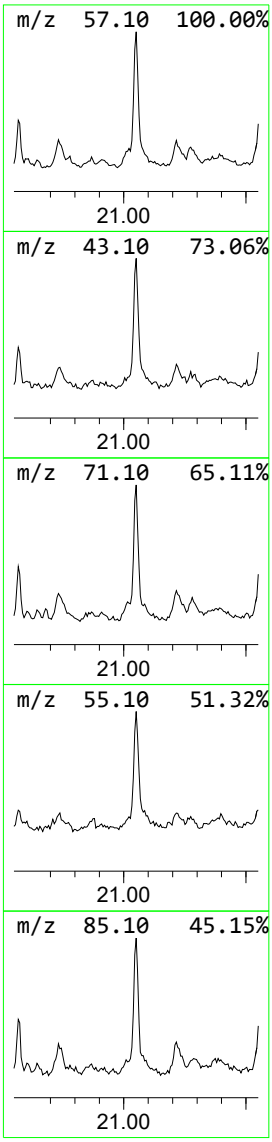
Peak Number 6 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	4.41 ng	893064	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	87





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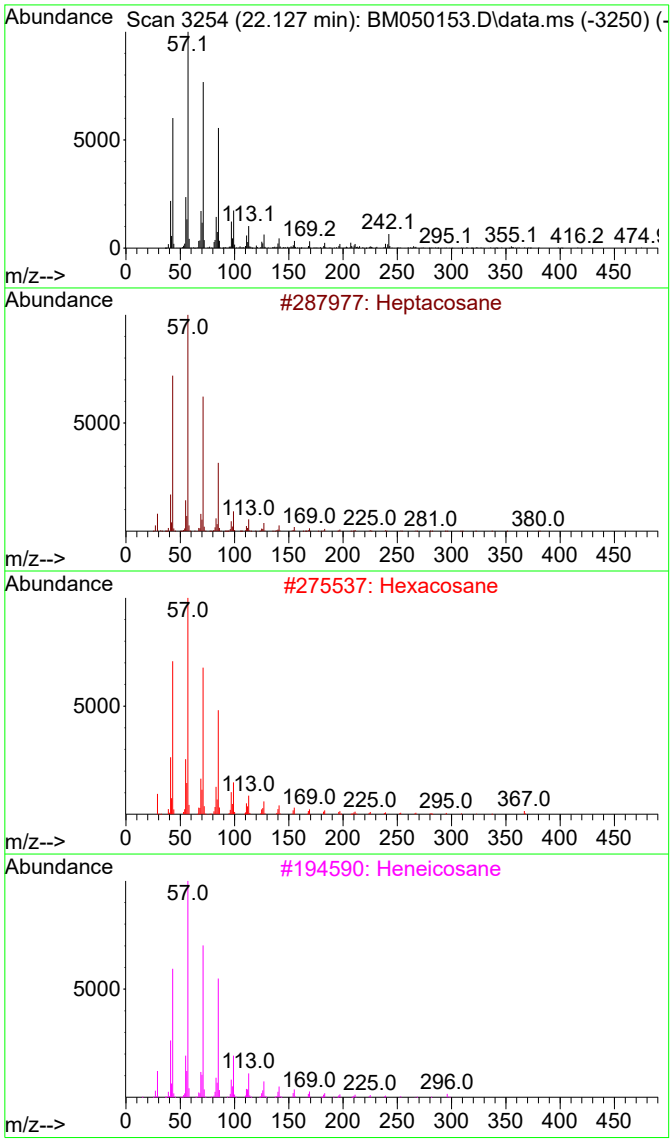
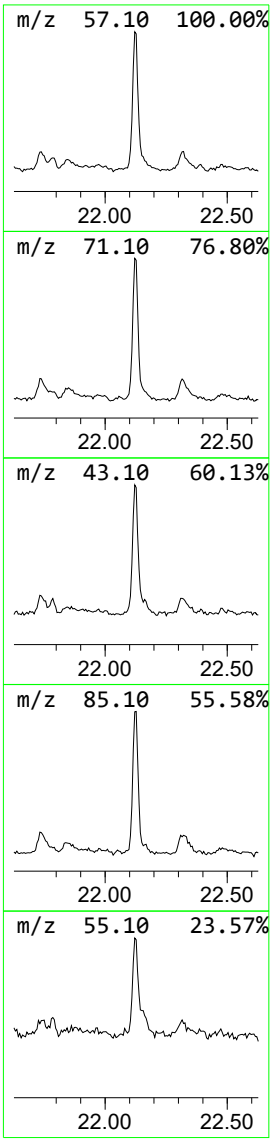
Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.127	4.47 ng	903596	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Tetracosane	338	C24H50	000646-31-1	90





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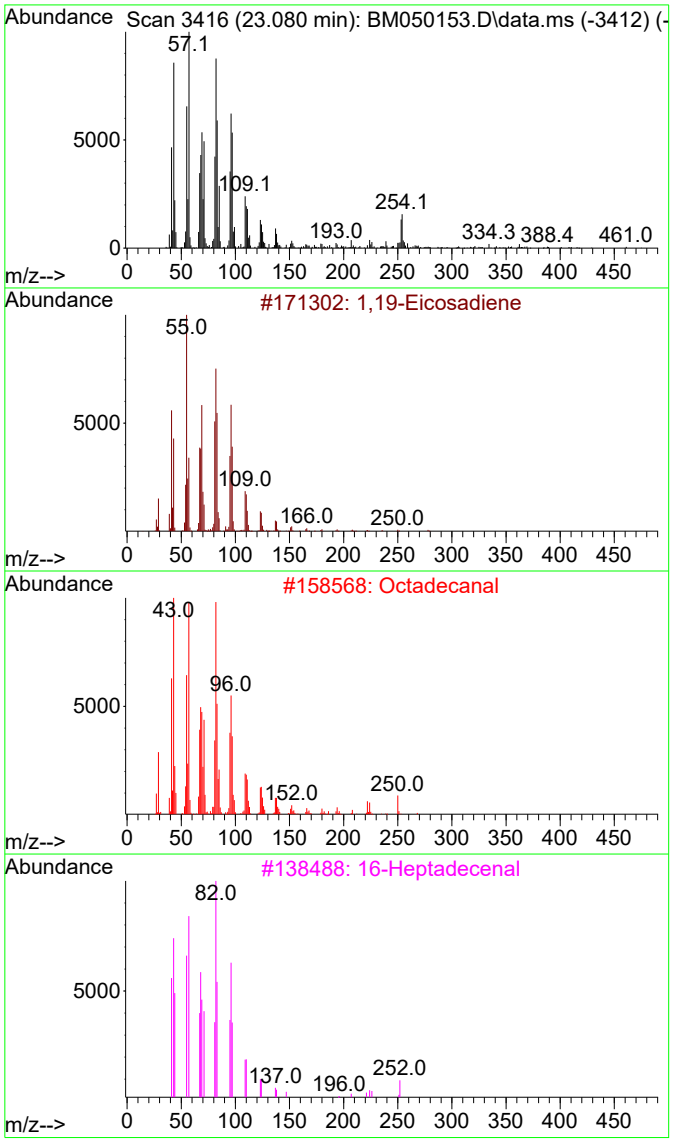
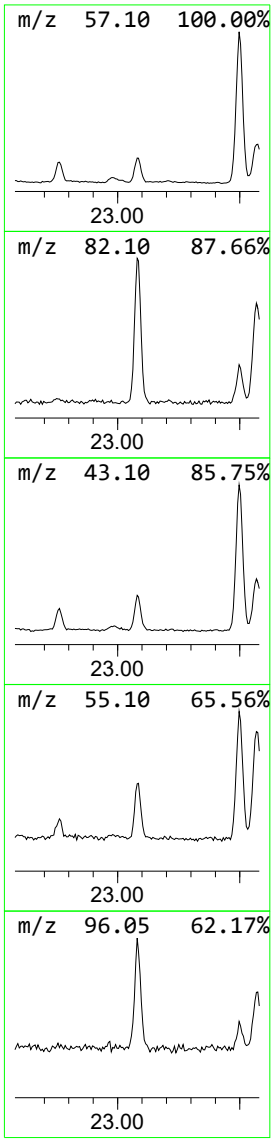
Peak Number 8 1,19-Eicosadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.080	4.35 ng	757272	Perylene-d12	24.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	94
2	Octadecanal	268	C18H36O	000638-66-4	94
3	16-Heptadecenal	252	C17H32O	1010144-57-9	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	89
5	Eicosanal-	296	C20H40O	002400-66-0	87





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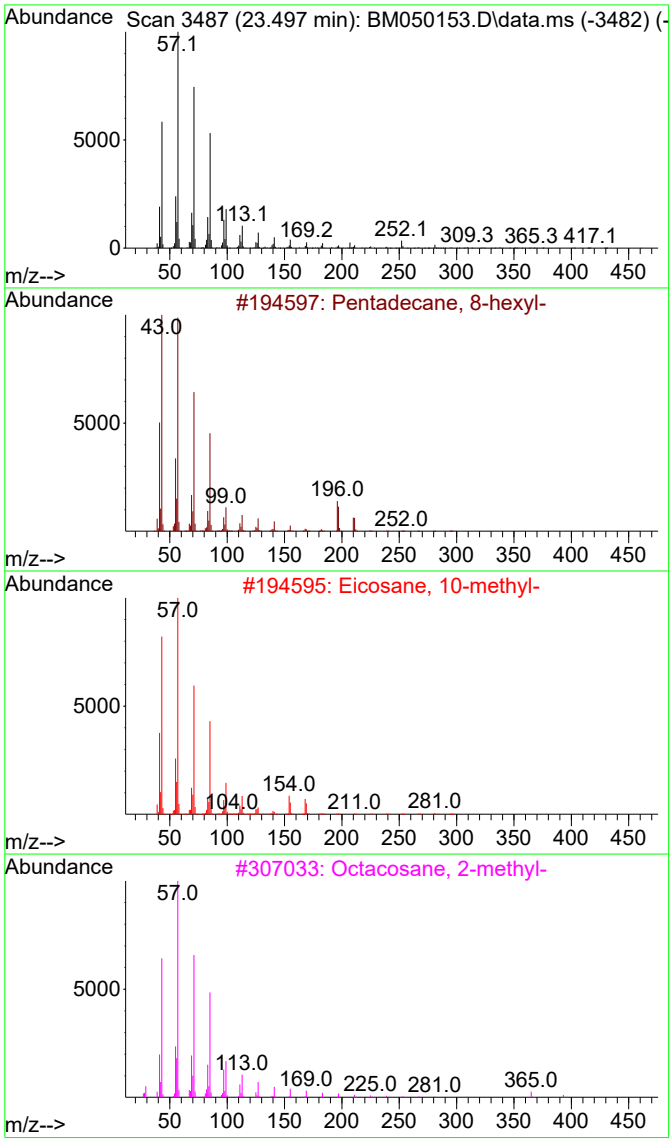
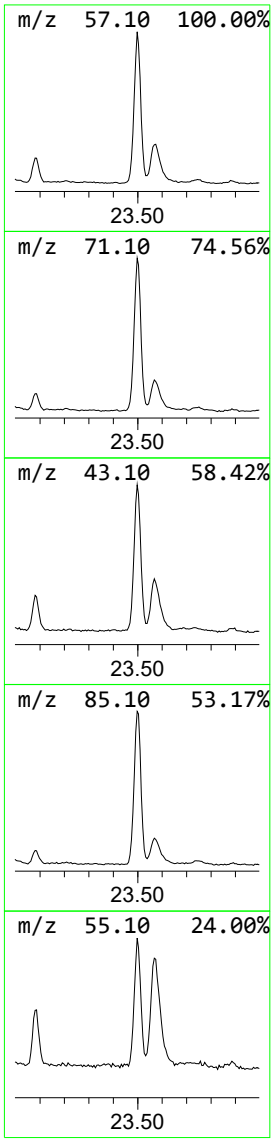
Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.497	12.91 ng	2248140	Perylene-d12	24.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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Acq On : 08 May 2025 19:17
Operator : RC/JU
Sample : Q1972-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-B-1

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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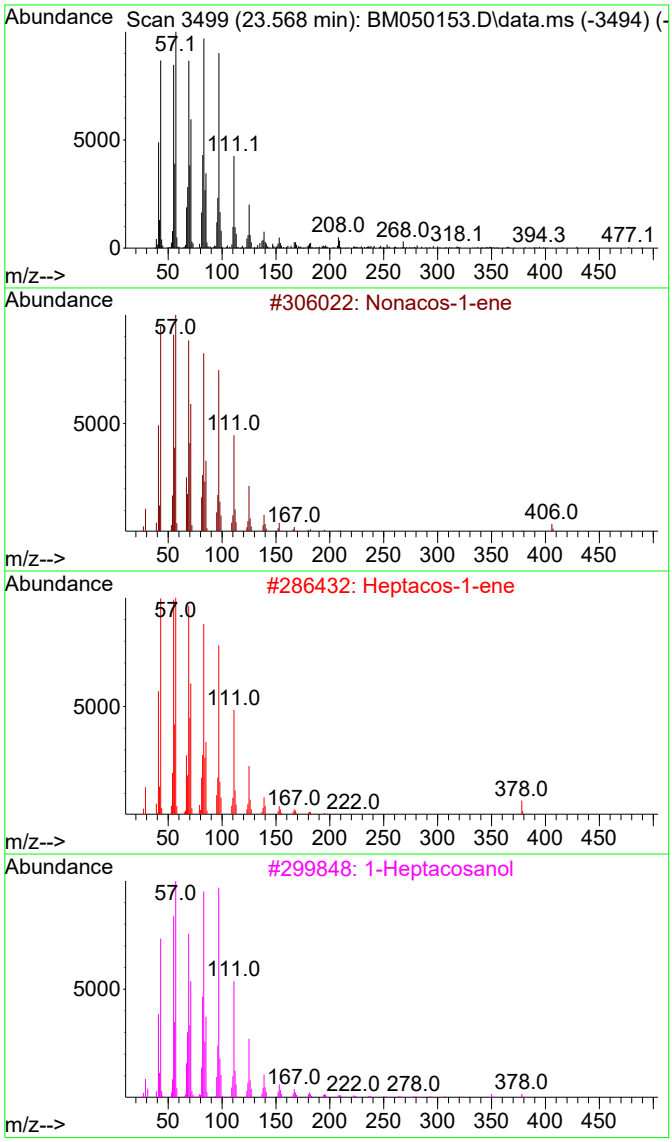
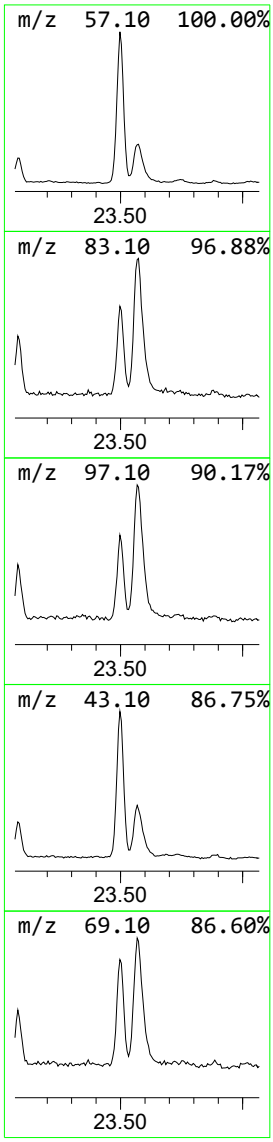
Peak Number 10 Nonacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.568	8.55 ng	1489060	Perylene-d12	24.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Triacontan-15-ol	438	C30H62O	031849-26-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050153.D
Acq On : 08 May 2025 19:17
Operator : RC/JU
Sample : Q1972-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-B-1

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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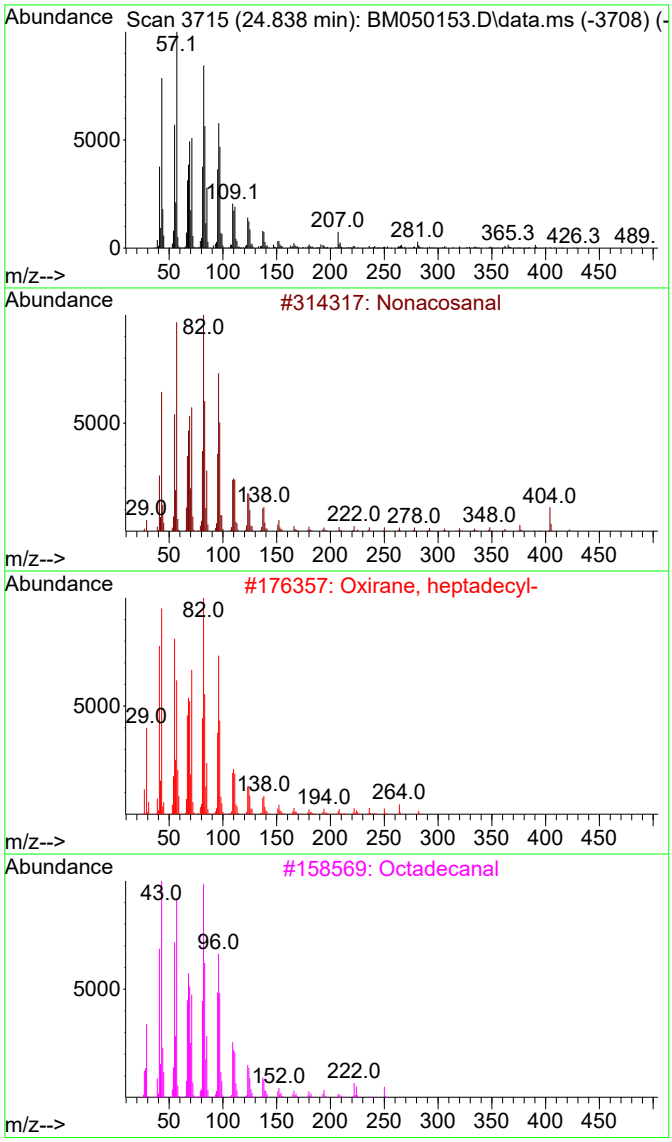
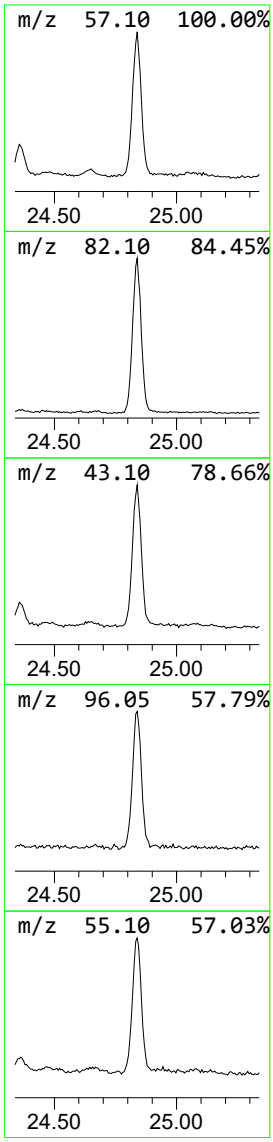
Peak Number 11 Nonacosanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.838	14.85 ng	2586590	Perylene-d12	24.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosanal	422	C29H58O	072934-04-4	95
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	Octacosanal	408	C28H56O	022725-64-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050153.D
Acq On : 08 May 2025 19:17
Operator : RC/JU
Sample : Q1972-21
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-B-1

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	3.487	2.6	ng	198497	1	7.740	1551930	20.0
2-Pentanone, 4-...	4.863	4.7	ng	363398	1	7.740	1551930	20.0
1-Phenoxypropan...	11.310	2.1	ng	213789	2	10.534	2029730	20.0
n-Hexadecanoic ...	18.039	8.2	ng	1328950	4	17.139	3257920	20.0
Octadecanoic acid	19.315	2.6	ng	518982	5	21.380	4045950	20.0
1-Docosene	21.051	4.4	ng	893064	5	21.380	4045950	20.0
Heptacosane	22.127	4.5	ng	903596	5	21.380	4045950	20.0
1,19-Eicosadiene	23.080	4.3	ng	757272	6	24.374	3483350	20.0
Pentadecane, 8-...	23.497	12.9	ng	2248140	6	24.374	3483350	20.0
Nonacos-1-ene	23.568	8.6	ng	1489060	6	24.374	3483350	20.0
Nonacosanal	24.838	14.9	ng	2586590	6	24.374	3483350	20.0