LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121021\
Data File : BM033394.D
Acq On : 10 Dec 2021 15:01
Operator : CG/JU
Sample : M4919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

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-BM120821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.490	376	383	391	rBV	572203	851218	19.61%	2.217%
2	7.078	646	653	662	rBV	337481	550800	12.69%	1.435%
3	7.901	787	793	800	rBV	247023	402744	9.28%	1.049%
4	9.066	983	991	998	rBV	974177	1624410	37.42%	4.231%
5	10.701	1261	1269	1274	rBV	332718	602614	13.88%	1.569%
6	13.154	1679	1686	1692	rBV	2269419	3346521	77.09%	8.716%
7	14.530	1914	1920	1925	rBV	540441	791466	18.23%	2.061%
8	14.583	1925	1929	1936	rVB	41495	68645	1.58%	0.179%
9	15.089	2010	2015	2032	rVB2	130121	273634	6.30%	0.713%
10	15.860	2141	2146	2157	rVB3	47573	142362	3.28%	0.371%
11	15.966	2160	2164	2167	rVV	63679	91700	2.11%	0.239%
12	16.018	2167	2173	2180	rVB	2097342	3028980	69.77%	7.889%
13	16.301	2215	2221	2232	rVB2	182392	331695	7.64%	0.864%
14	16.565	2261	2266	2271	rBV	81243	131821	3.04%	0.343%
15	16.660	2275	2282	2295	rVB2	366077	721447	16.62%	1.879%
16	16.813	2304	2308	2320	rVB	101142	180982	4.17%	0.471%
17	17.271	2380	2386	2391	rBV	719747	1080754	24.90%	2.815%
18	17.924	2494	2497	2503	rVB5	45978	60802	1.40%	0.158%
19	18.154	2531	2536	2546	rBV	172418	292759	6.74%	0.762%
20	18.442	2579	2585	2589	rBV	800372	1345644	31.00%	3.505%
21	18.489	2589	2593	2606	rVB	1159030	1912895	44.06%	4.982%
22	18.683	2613	2626	2640	rVB2	508112	2201592	50.71%	5.734%
23	19.424	2749	2752	2764	rVB2	94393	135221	3.11%	0.352%
24	19.883	2824	2830	2835	rBV	3365232	4341147	100.00%	11.306%
25	20.101	2858	2867	2877	rBV2	845462	2548721	58.71%	6.638%
26	21.077	3025	3033	3040	rBV	1111050	2372604	54.65%	6.179%
27	21.430	3088	3093	3105	rBV	872021	1160474	26.73%	3.022%
28	21.883	3162	3170	3177	rVB	917904	2171486	50.02%	5.656%
29	21.959	3179	3183	3190	rVB4	110495	216598	4.99%	0.564%
30	22.753	3311	3318	3328	rVB	832849	1945078	44.81%	5.066%
31	23.747	3479	3487	3500	rVB3	922437	2399864	55.28%	6.250%
32	24.894	3675	3682	3695	rVB2	349453	1069304	24.63%	2.785%

Sum of corrected areas: 38395982

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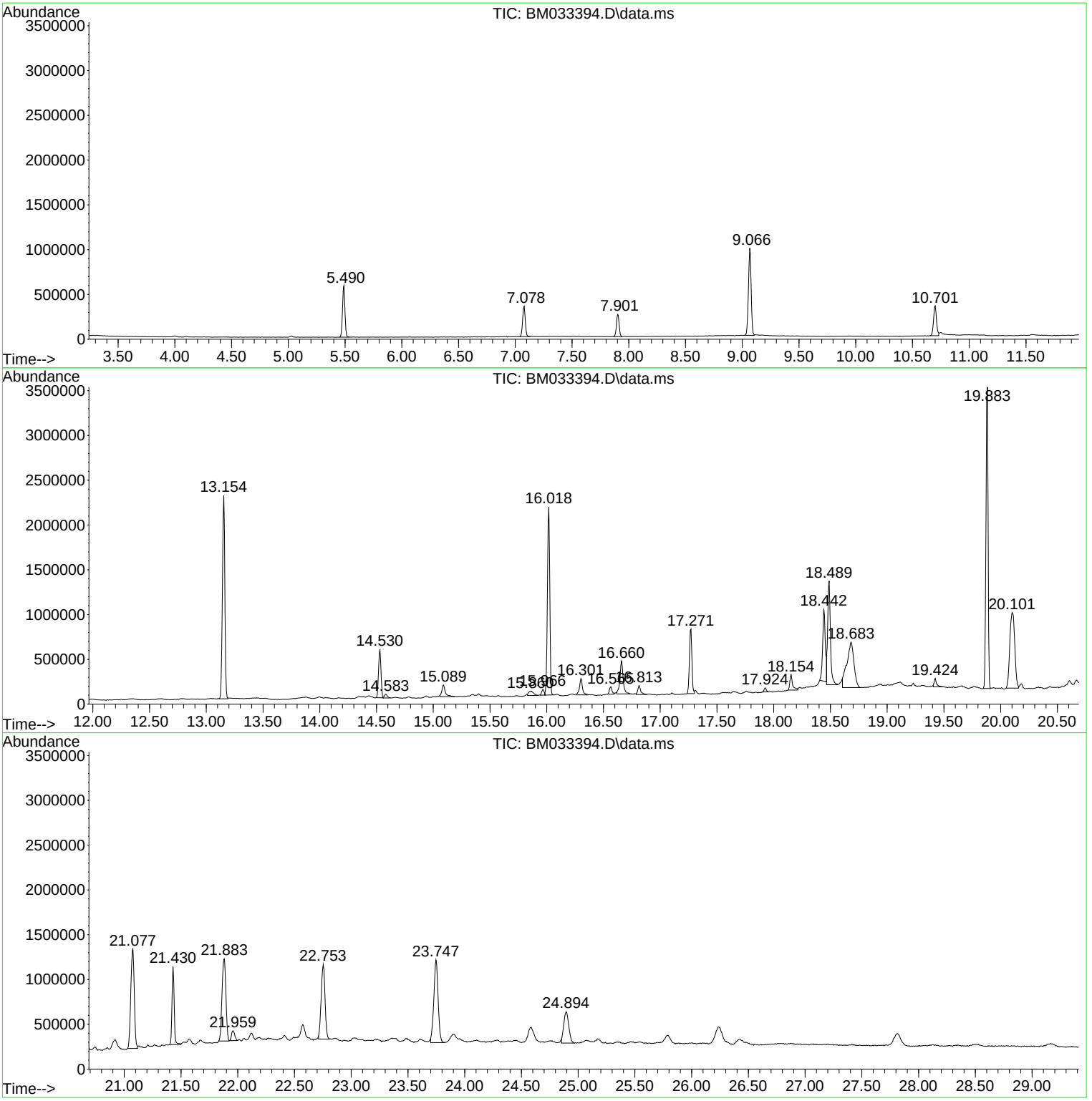
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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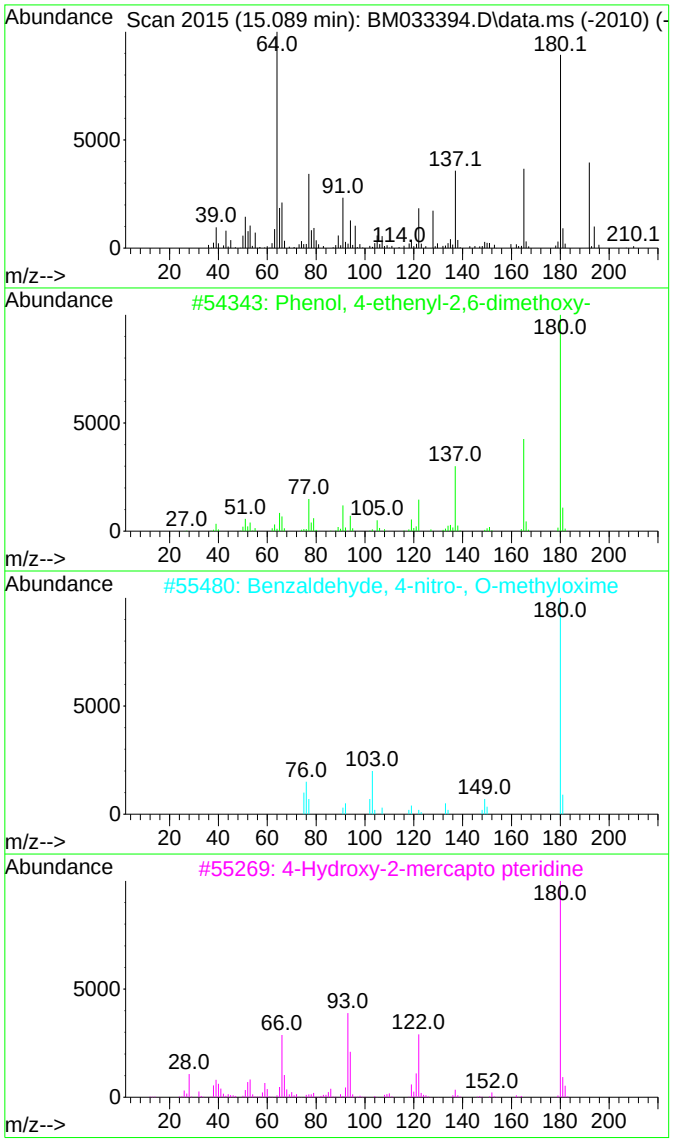
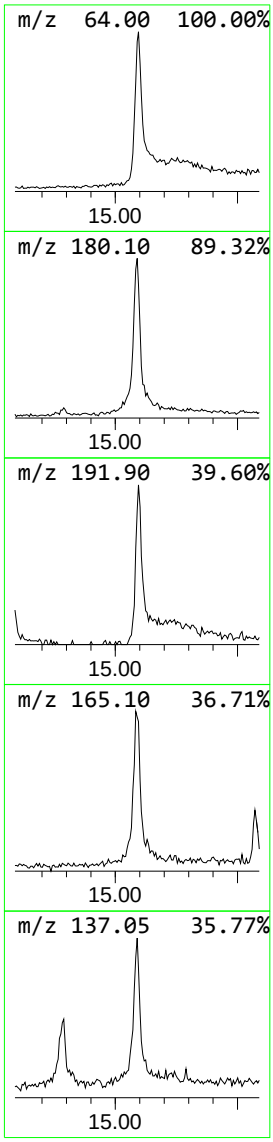
****
Peak Number 1 Phenol, 4-ethenyl-2,6-dimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.089	6.91 ng	273634	Acenaphthene-d10	14.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethenyl-2,6-dimethoxy-	180	C10H12O3	028343-22-8	53
2	Benzaldehyde, 4-nitro-, O-methyl...	180	C8H8N2O3	033499-32-0	25
3	4-Hydroxy-2-mercapto pteridine	180	C6H4N4OS	052023-48-0	18
4	Benzaldehyde, m-nitro-, O-methyl...	180	C8H8N2O3	033499-33-1	17
5	2,3,5,6-Tetrafluoroanisole	180	C7H4F4O	002324-98-3	11





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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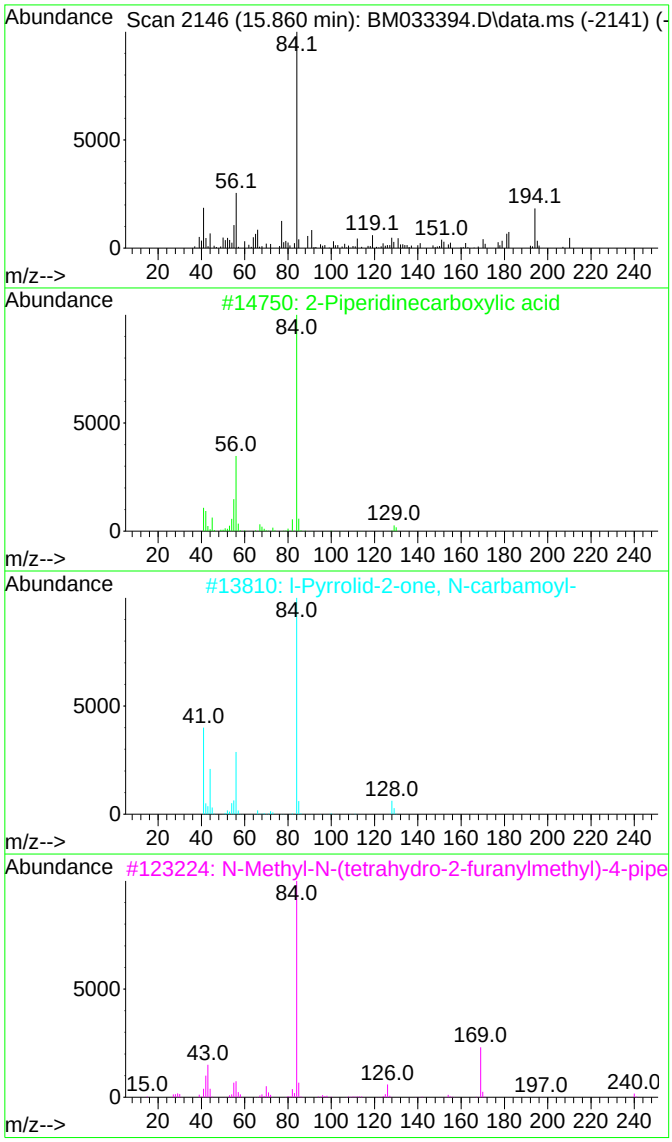
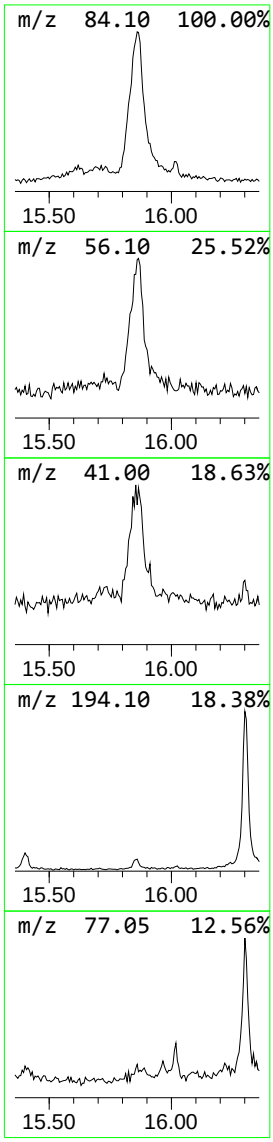
****

Peak Number 2 2-Piperidinecarboxylic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.860	3.60 ng	142362	Acenaphthene-d10	14.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinecarboxylic acid	129	C6H11NO2	000535-75-1	53
2	l-Pyrrolid-2-one, N-carbamoyl-	128	C5H8N2O2	040451-67-0	53
3	N-Methyl-N-(tetrahydro-2-furanyl...	240	C13H24N2O2	1000469-58-6	50
4	2-piperidineacetic acid, ethyl e...	171	C9H17NO2	1000404-61-1	50
5	2-Nonylcyclopentanone	210	C14H26O	1000433-19-9	47





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ClientSampleId :
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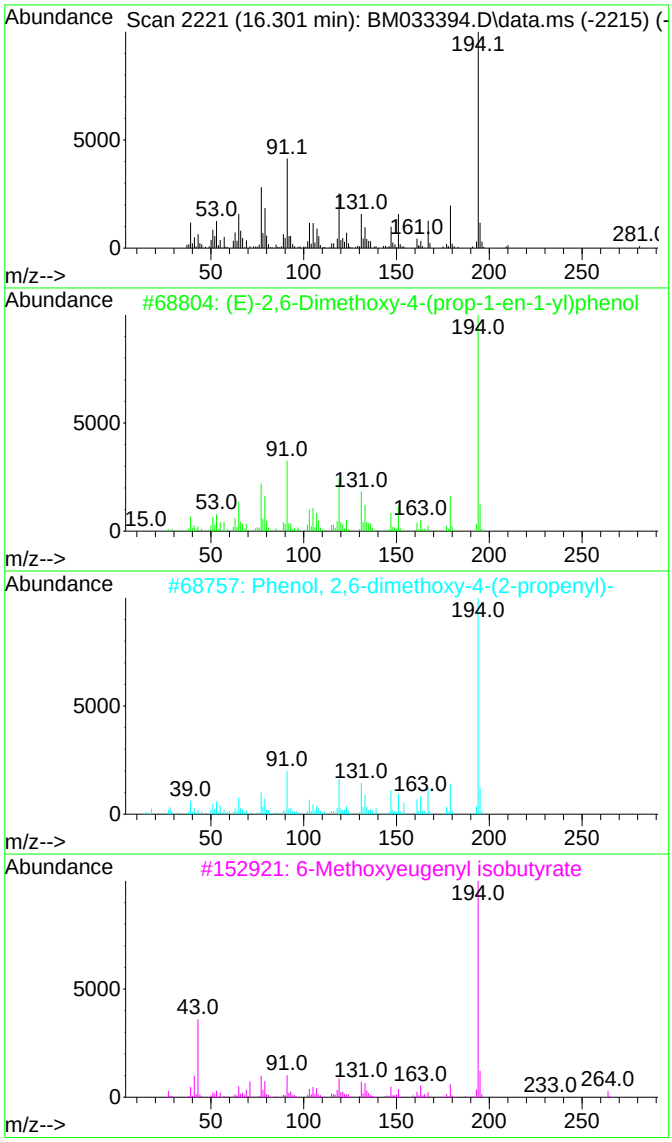
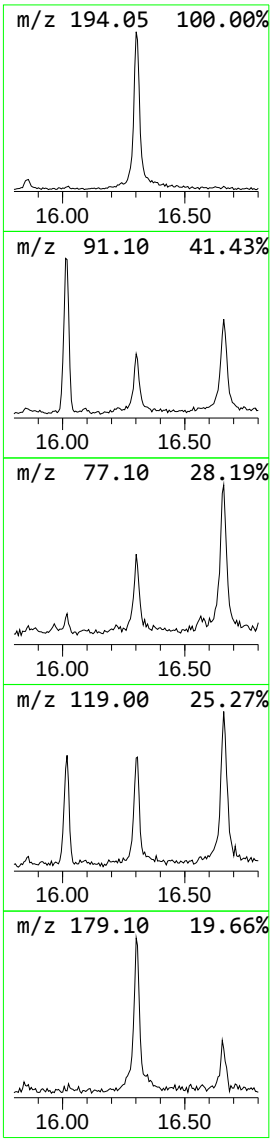
****
Peak Number 3 (E)-2,6-Dimethoxy-4-(prop-1... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.301	6.14 ng	331695	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-2,6-Dimethoxy-4-(prop-1-en-1...	194	C11H14O3	020675-95-0	94
2	Phenol, 2,6-dimethoxy-4-(2-prope...	194	C11H14O3	006627-88-9	94
3	6-Methoxyeugenyl isobutyrate	264	C15H20O4	1000465-70-7	64
4	2-Propenoic acid, 3-(4-hydroxy-3...	194	C10H10O4	001135-24-6	52
5	3-Hydroxy-4-methoxycinnamic acid	194	C10H10O4	000537-73-5	52





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Operator : CG/JU
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
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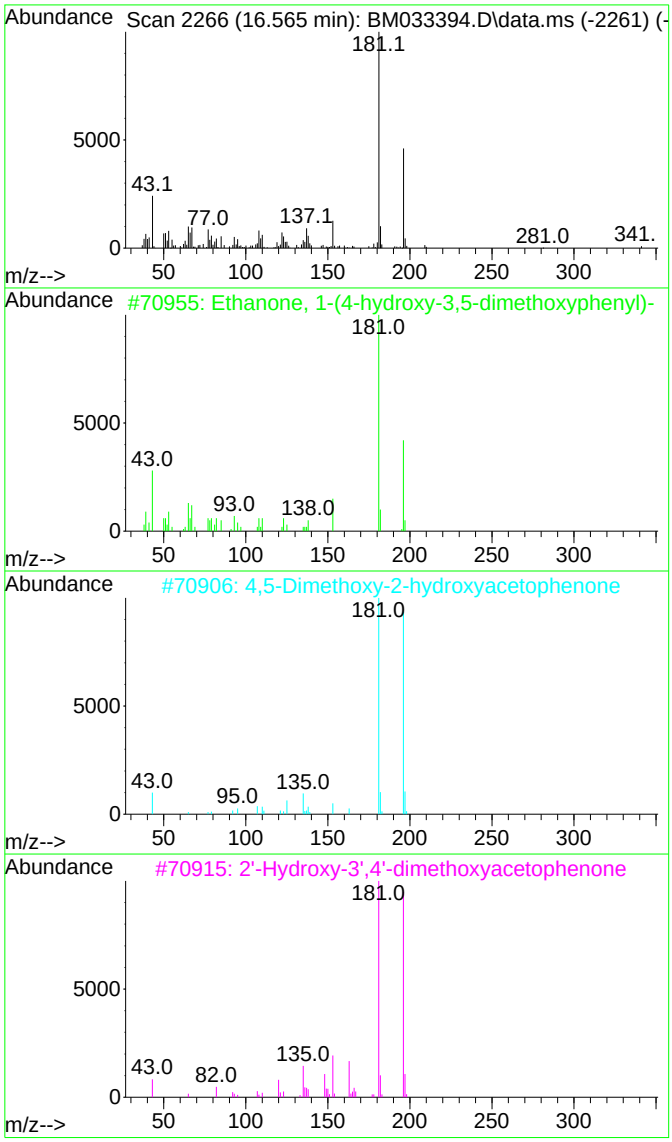
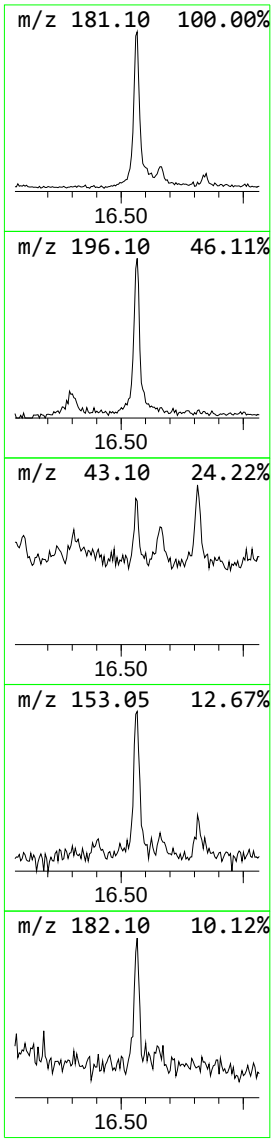
****

Peak Number 4 Ethanone, 1-(4-hydroxy-3,5-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.566	2.44 ng	131821	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	97
2	4,5-Dimethoxy-2-hydroxyacetophenone	196	C10H12O4	020628-06-2	87
3	2'-Hydroxy-3',4'-dimethoxyacetop...	196	C10H12O4	1000433-07-2	80
4	4-Acetyl-2,6-dimethoxyphenyl ace...	238	C12H14O5	1000385-76-7	74
5	3'-Hydroxy-2',4'-dimethoxyacetop...	196	C10H12O4	1000433-07-3	64





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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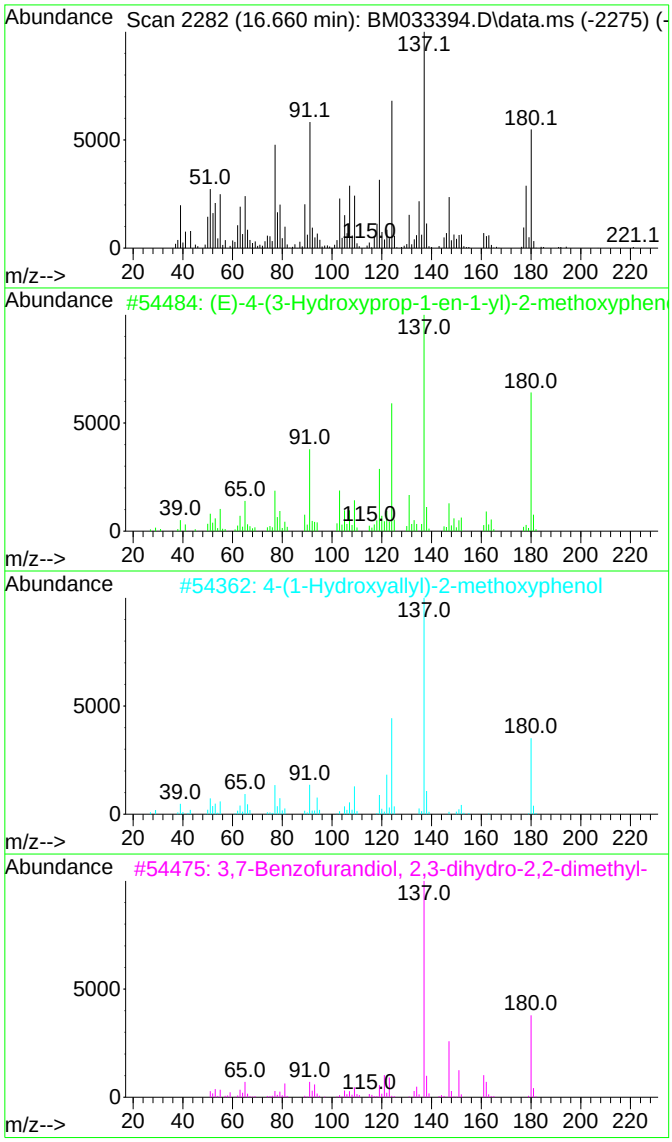
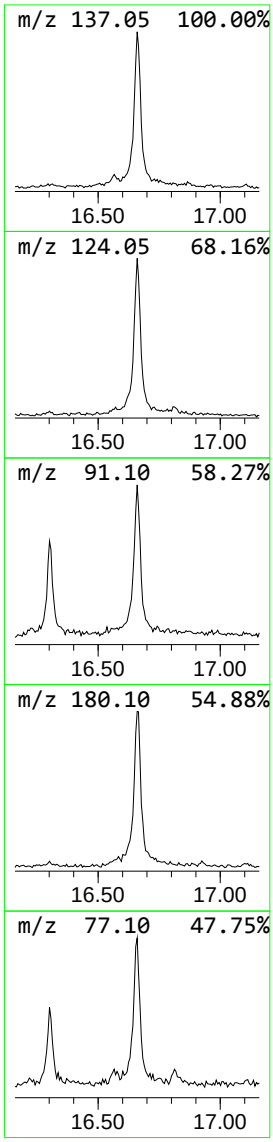
****
Peak Number 5 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.660	13.35 ng	721447	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	83
2	4-(1-Hydroxyallyl)-2-methoxyphenol	180	C10H12O3	112465-50-6	53
3	3,7-Benzofurandiol, 2,3-dihydro-...	180	C10H12O3	017781-15-6	43
4	Benzaldehyde, 2-hydroxy-, oxime	137	C7H7NO2	000094-67-7	38
5	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	38





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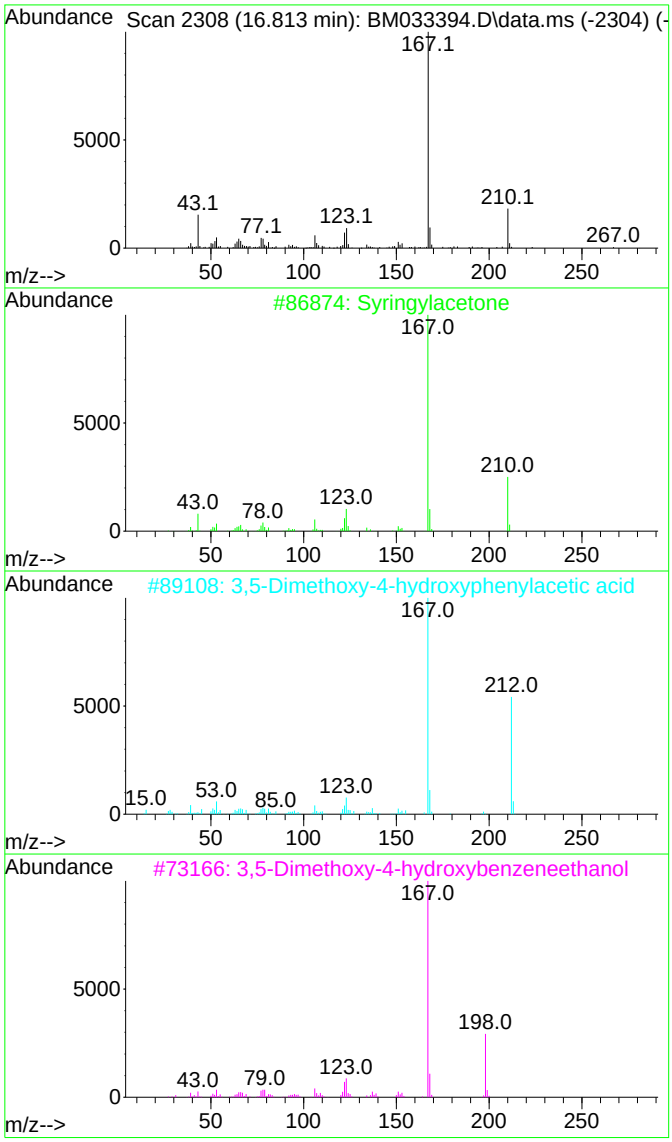
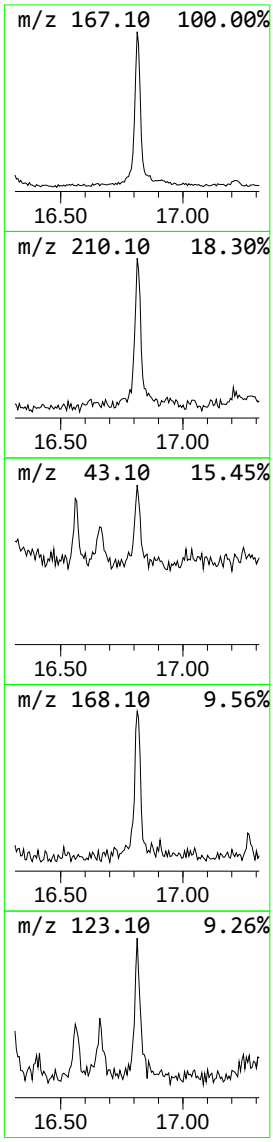
****

Peak Number 6 Syringylacetone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.813	3.35 ng	180982	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Syringylacetone	210	C11H14O4	019037-58-2	96
2	3,5-Dimethoxy-4-hydroxyphenylace...	212	C10H12O5	004385-56-2	80
3	3,5-Dimethoxy-4-hydroxybenzeneet...	198	C10H14O4	020824-45-7	72
4	2,6-Dimethoxy-4-propylphenol	196	C11H16O3	006766-82-1	72
5	1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	59





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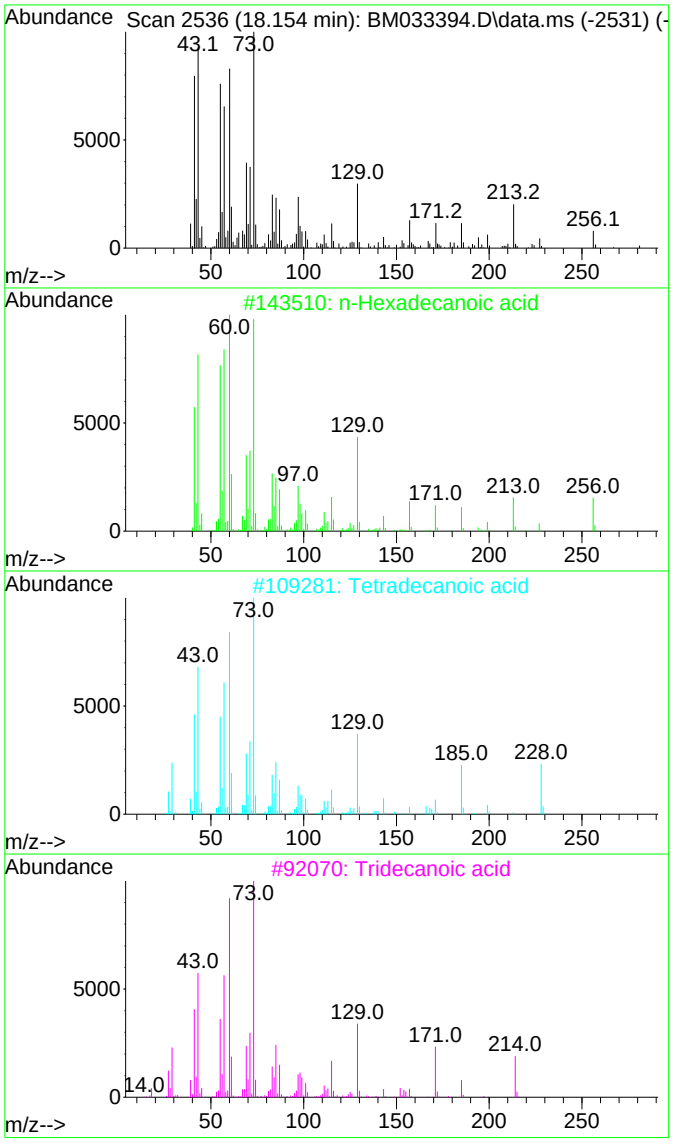
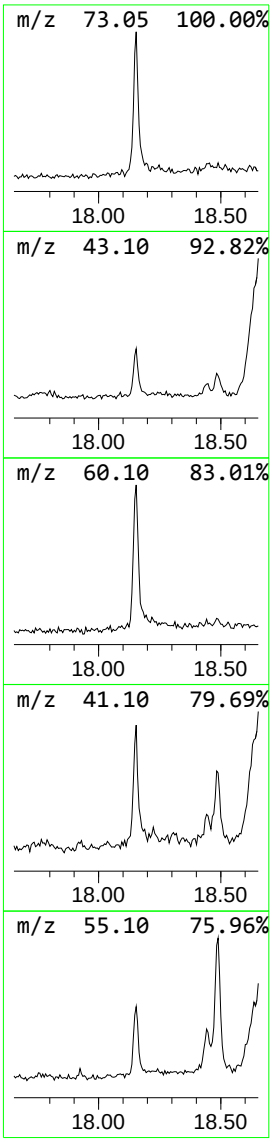
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.154	5.42 ng	292759	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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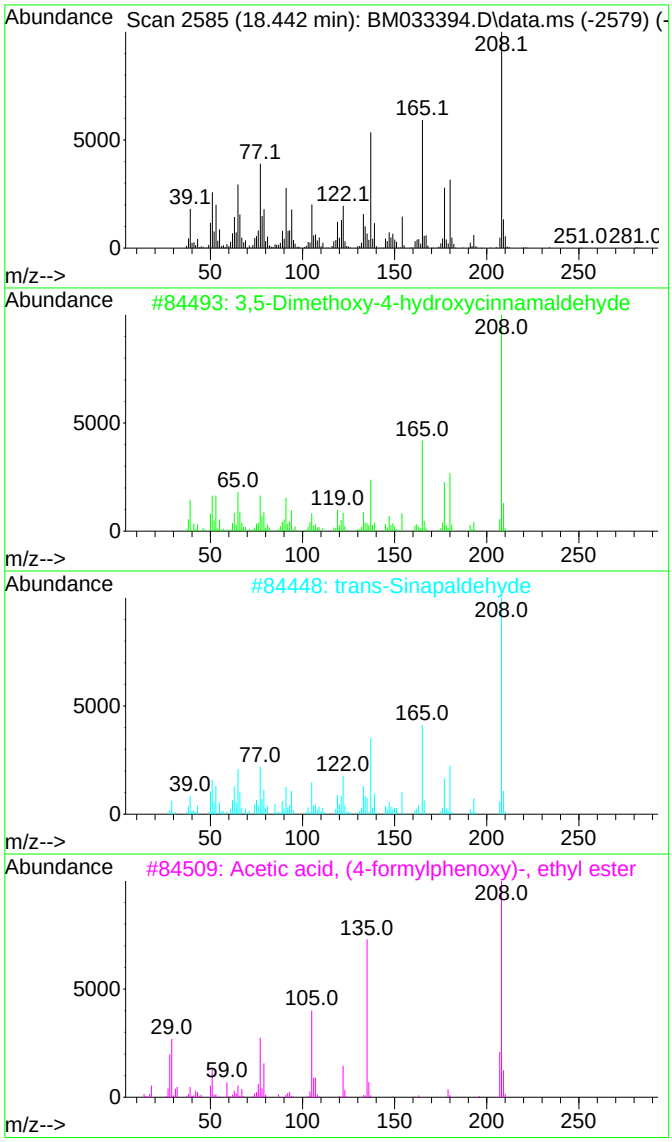
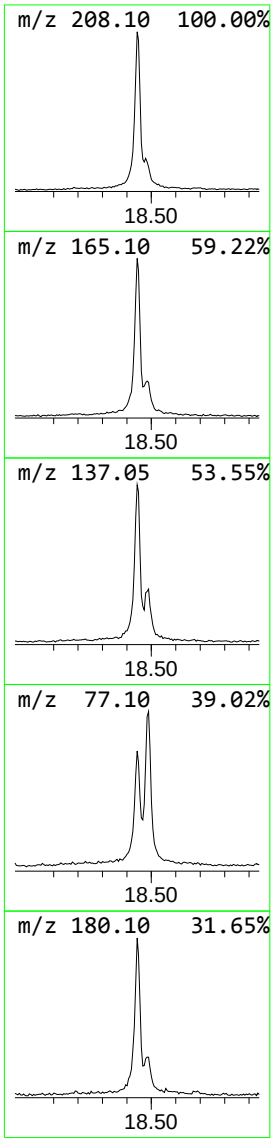
****
Peak Number 8 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.442	24.90 ng	1345640	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	96
2	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	91
3	Acetic acid, (4-formylphenoxy)-,...	208	C11H12O4	051264-69-8	46
4	1,3,4-Thiadiazolium, 2,3-dihydro...	208	C9H8N2S2	019703-86-7	41
5	6-Amino-2-(4-methylpiperidin-1-y...	208	C10H16N4O	1000388-65-9	38





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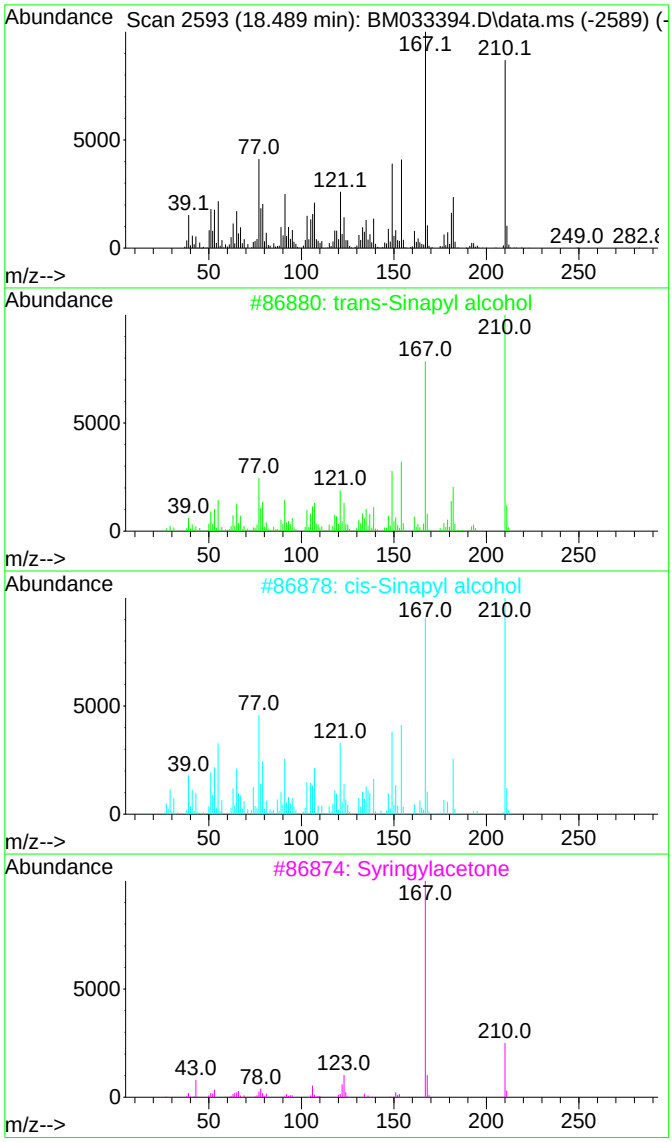
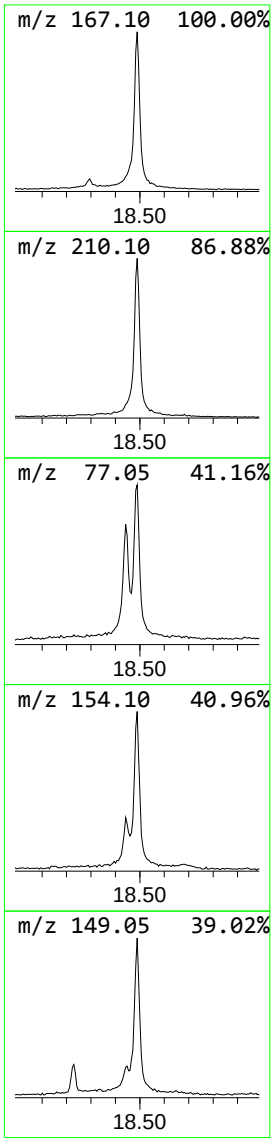
Peak Number 9 trans-Sinapyl alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	35.40 ng	1912900	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	96
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	93
3	Syringylacetone	210	C11H14O4	019037-58-2	50
4	4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	43
5	Phenol, 2-(2-imidazo[1,2-a]pyrid...	210	C13H10N2O	057636-32-5	38





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Data File : BM033394.D
Acq On : 10 Dec 2021 15:01
Operator : CG/JU
Sample : M4919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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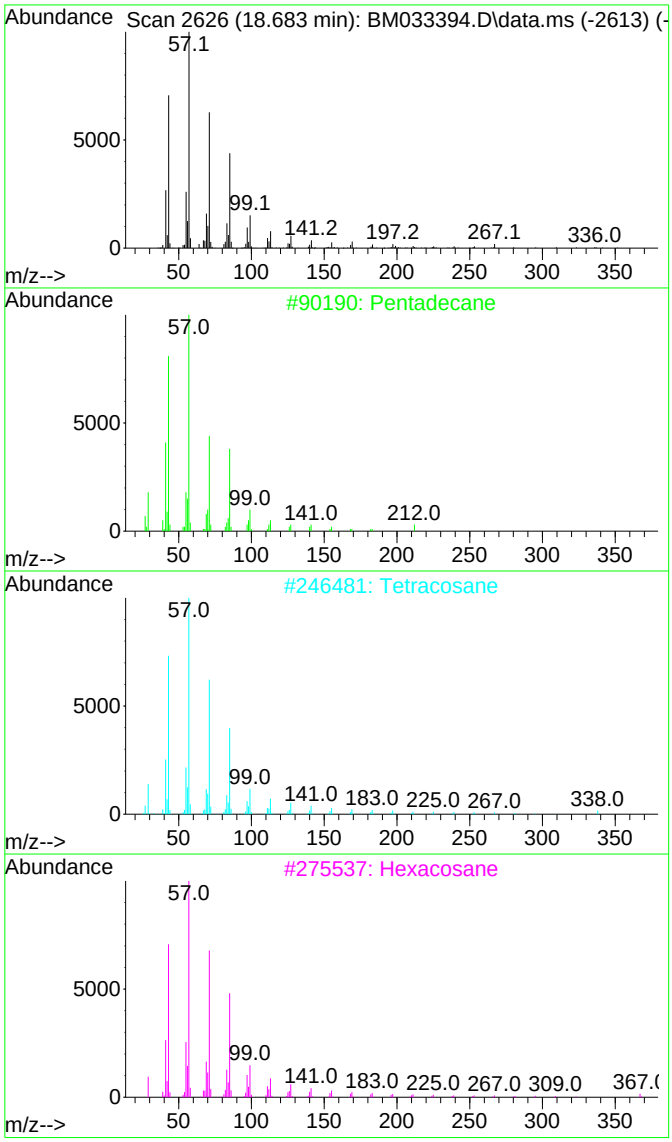
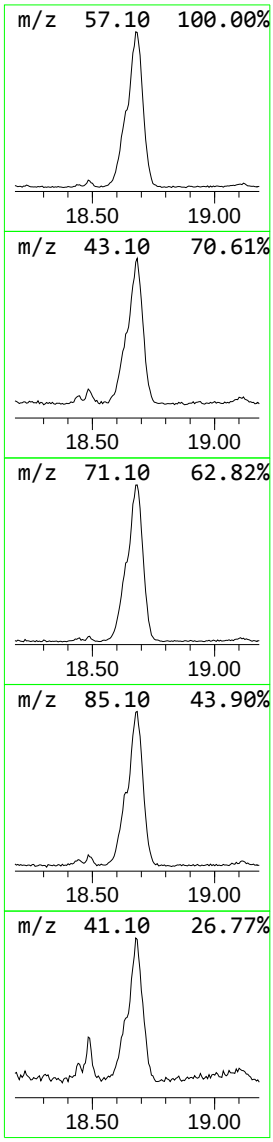
Peak Number 10 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.683	40.74 ng	2201590	Phenanthrene-d10	17.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Instrument :
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ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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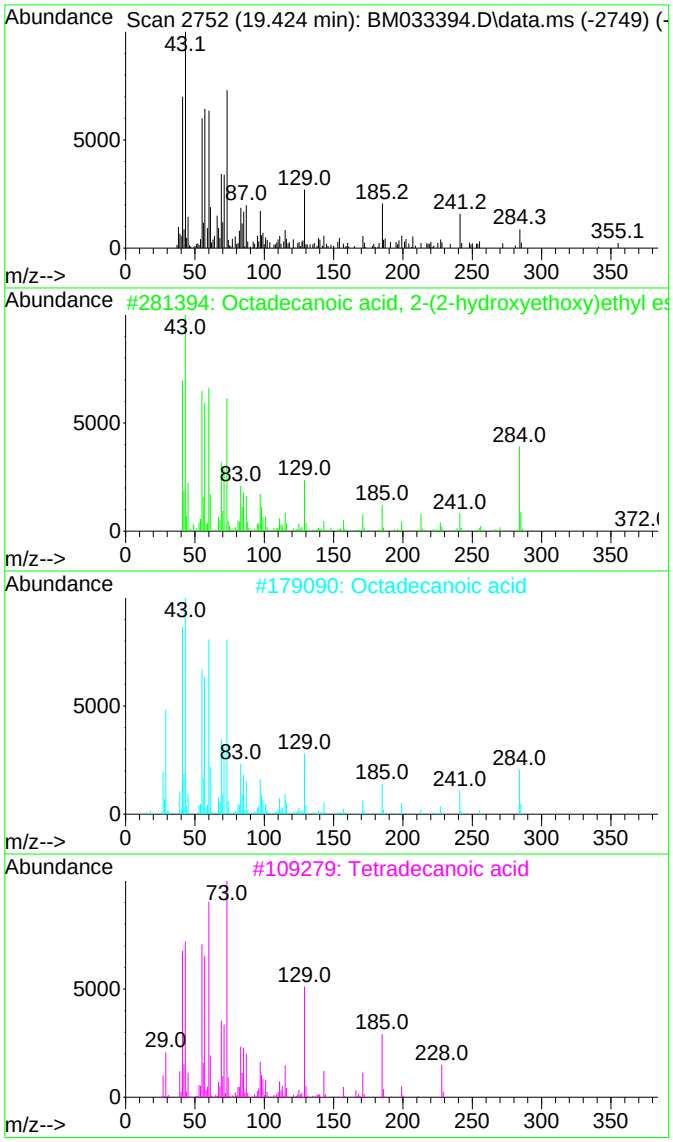
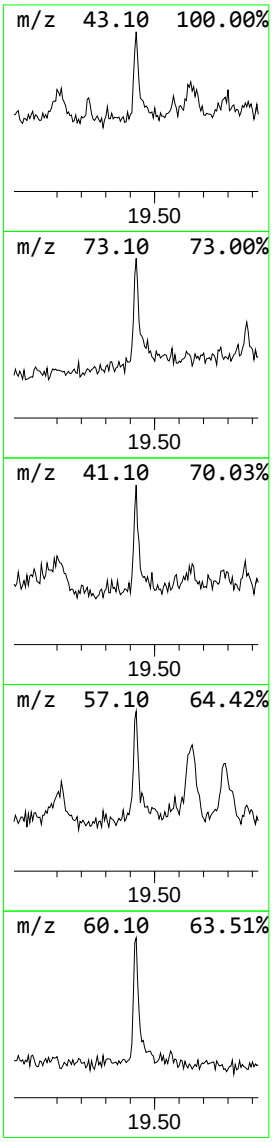
Peak Number 11 Octadecanoic acid, 2-(2-hyd... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.424	2.33 ng	135221	Chrysene-d12	21.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
2	Octadecanoic acid	284	C18H36O2	000057-11-4	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





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Sample : M4919-03
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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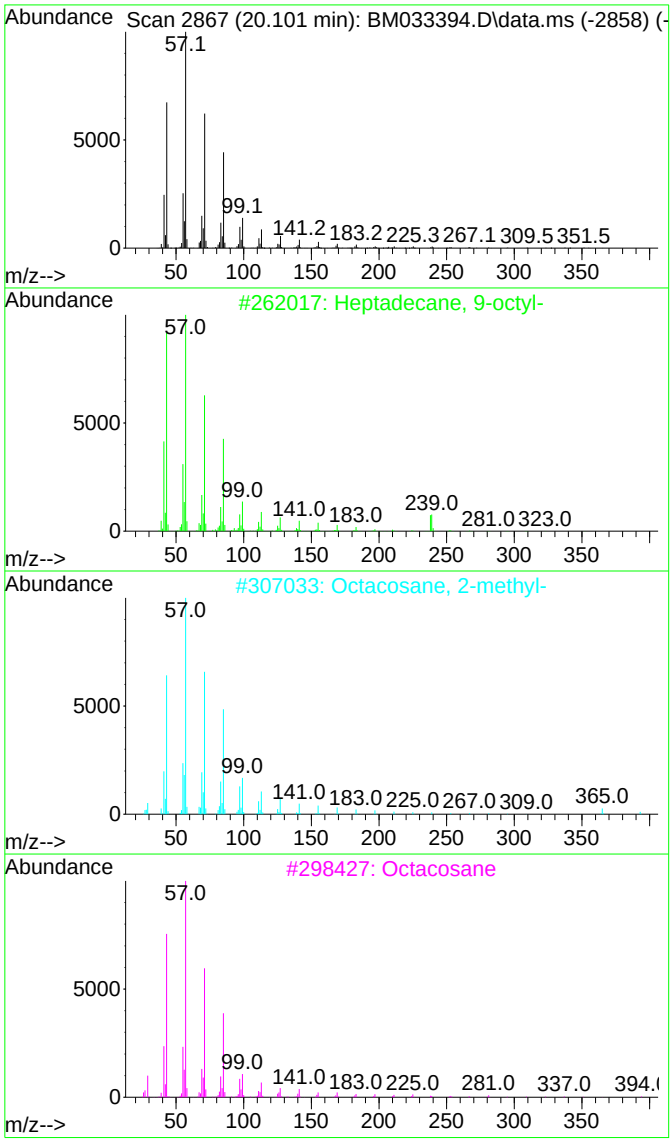
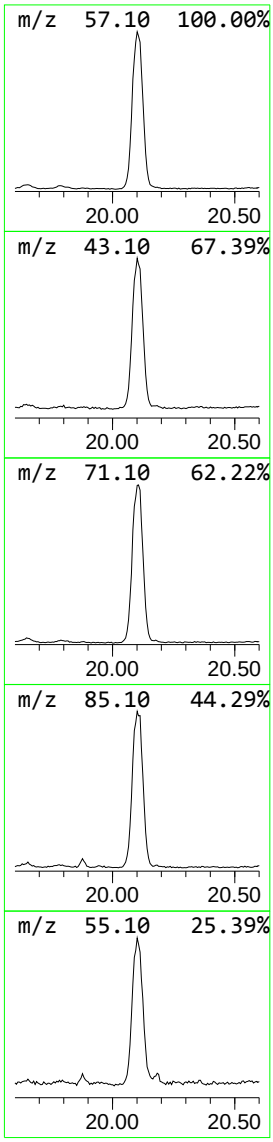
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.101	43.93 ng	2548720	Chrysene-d12	21.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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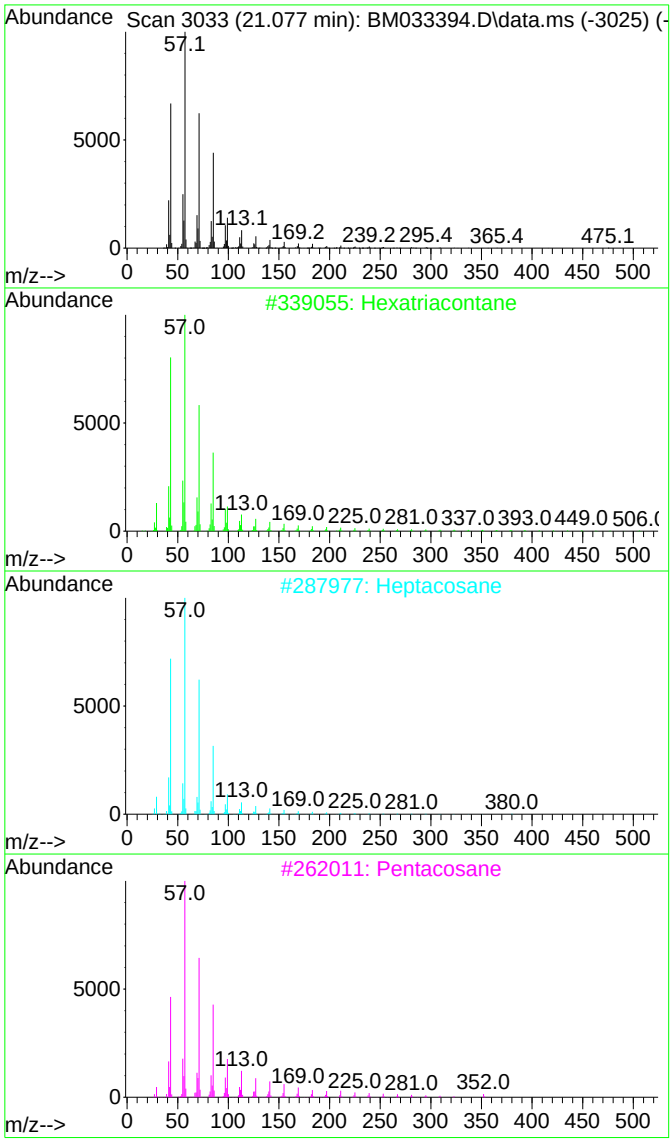
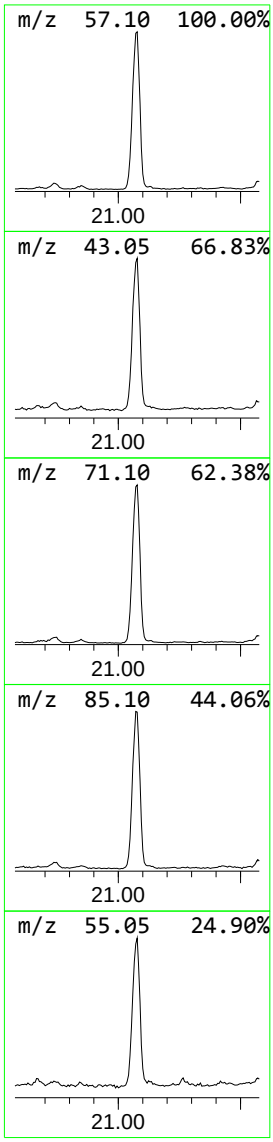
Peak Number 13 Hexatriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.077	40.89 ng	2372600	Chrysene-d12	21.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Sample : M4919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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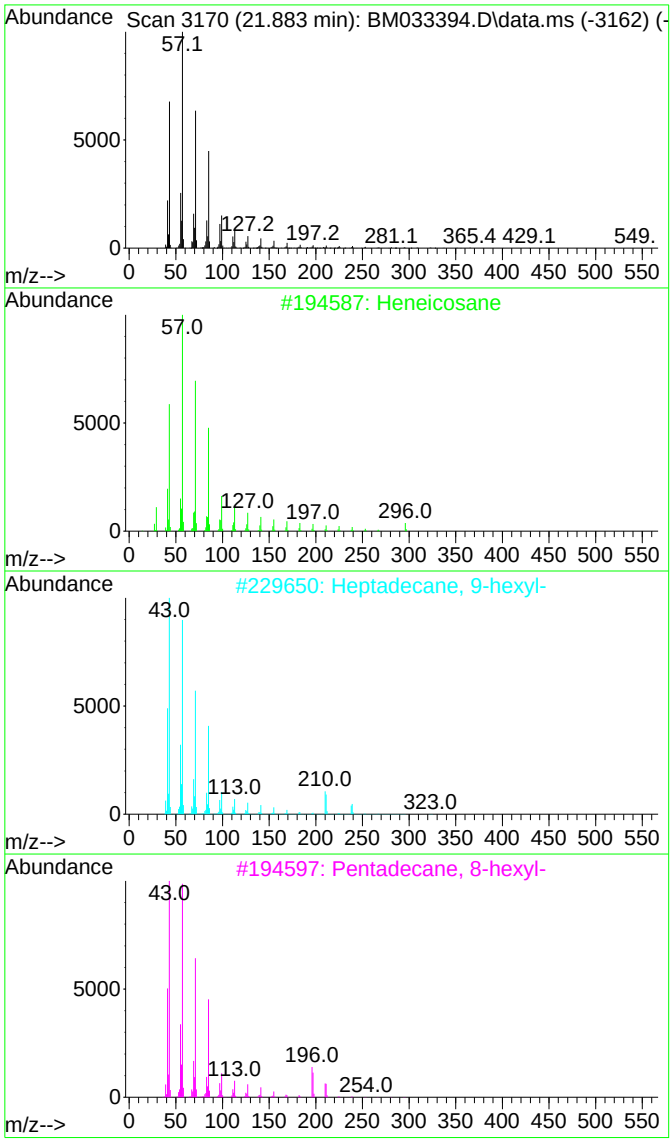
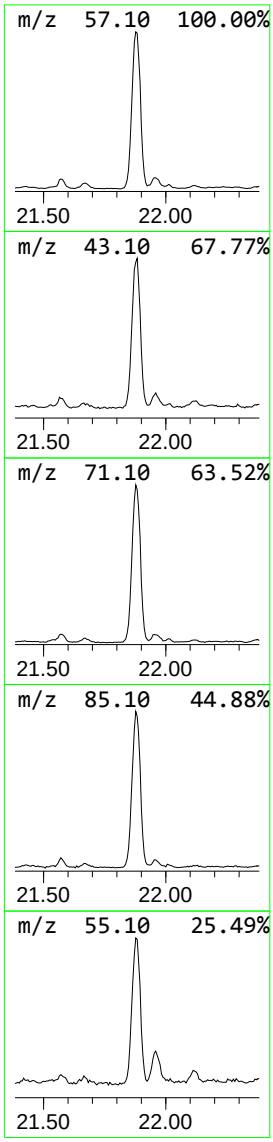
Peak Number 14 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.883	37.42 ng	2171490	Chrysene-d12	21.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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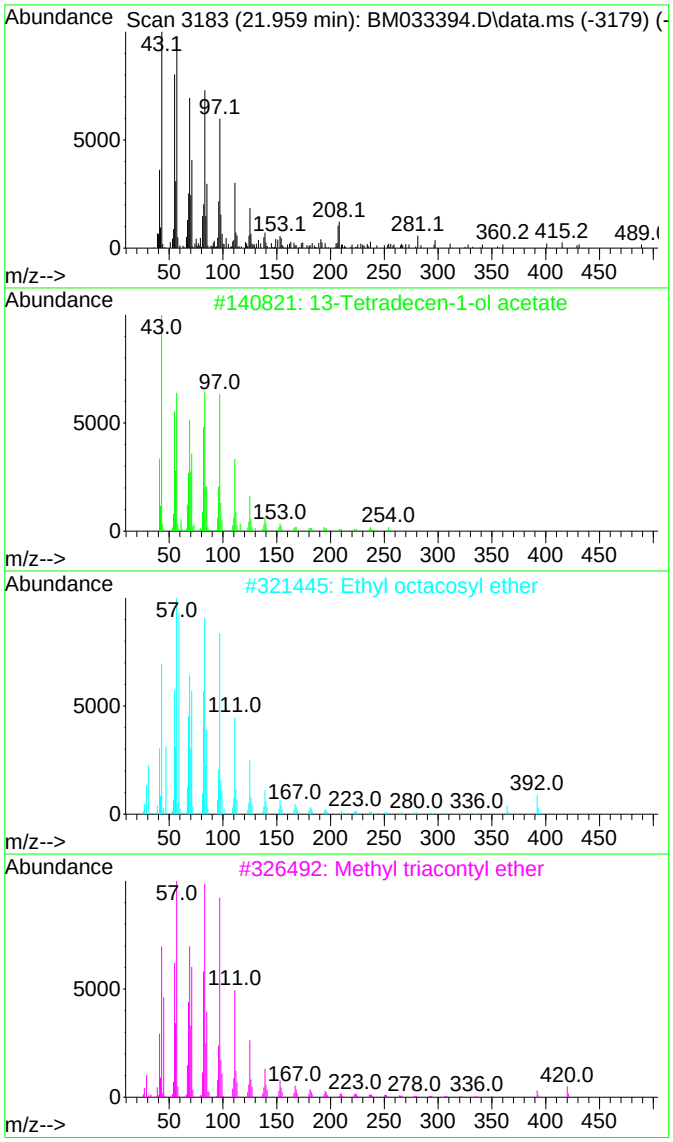
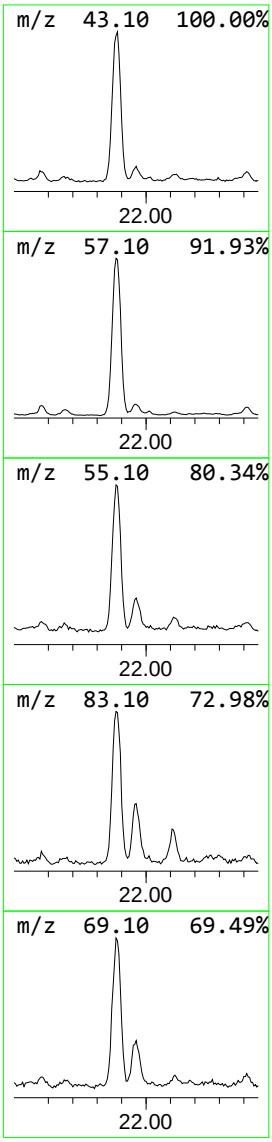
Peak Number 15 13-Tetradecen-1-ol acetate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.959	3.73 ng	216598	Chrysene-d12	21.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
2	Ethyl octacosyl ether	438	C30H62O	1010406-37-0	87
3	Methyl triacontyl ether	452	C31H64O	1000406-29-9	83
4	1-Methoxyoctacosane	424	C29H60O	237742-62-0	83
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





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Operator : CG/JU
Sample : M4919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.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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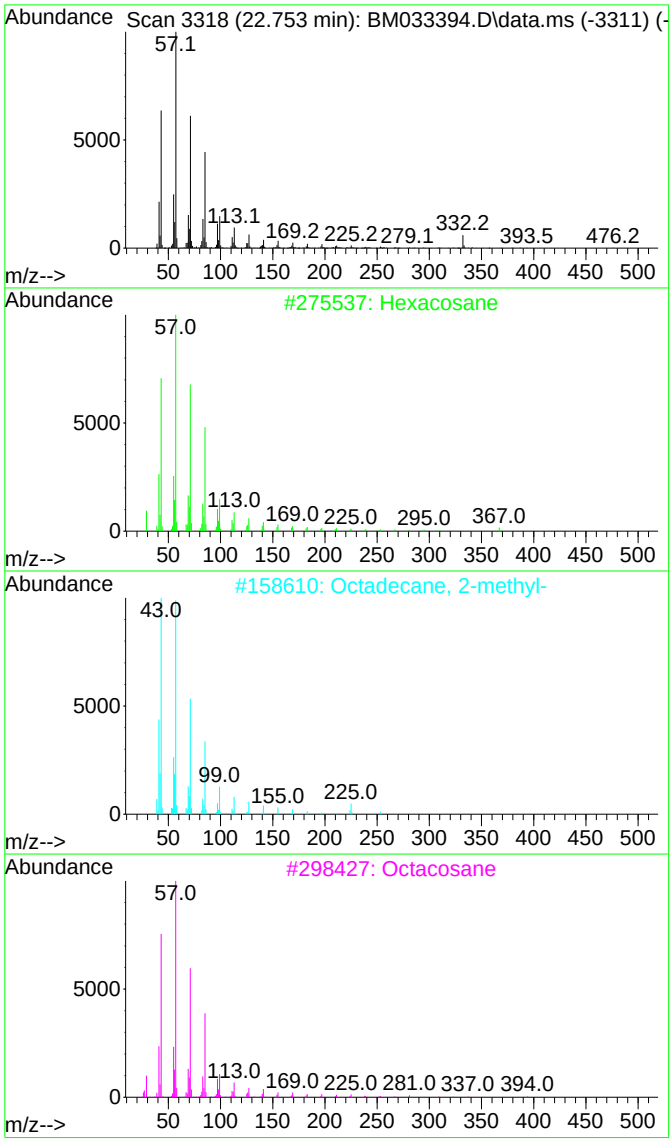
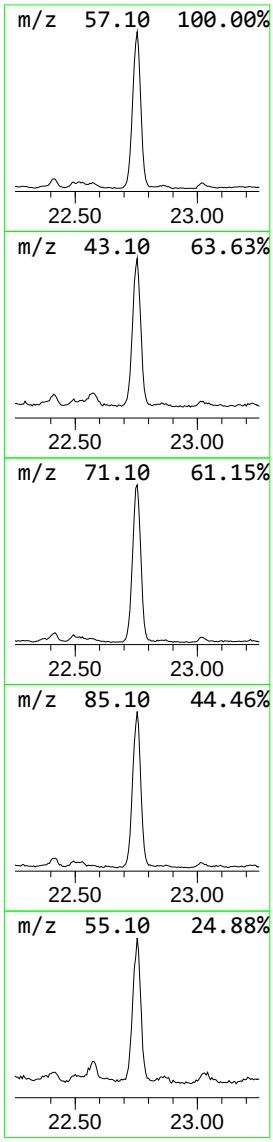
Peak Number 16 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.753	16.21 ng	1945080	Perylene-d12	23.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Sample : M4919-03
Misc :
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Instrument :
BNA_M
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FDR-MW-4-20211202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM120821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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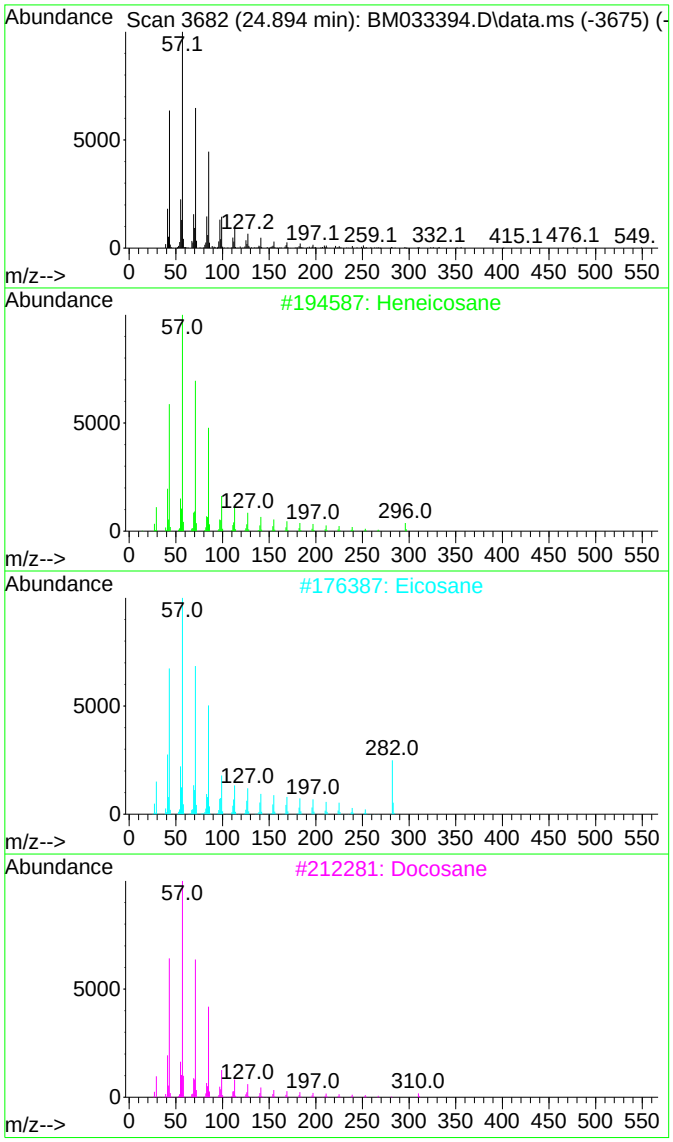
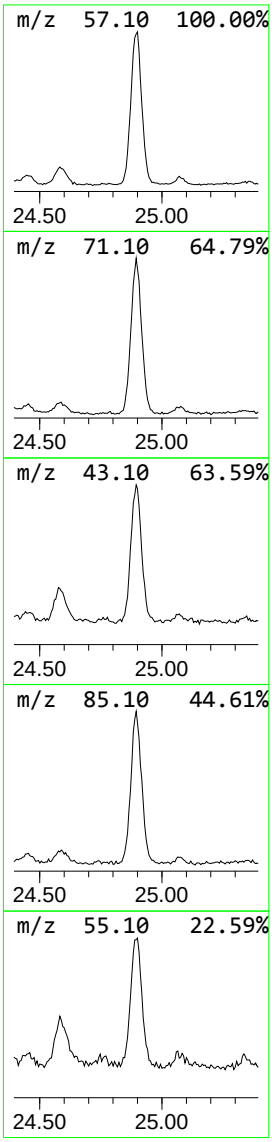
Peak Number 17 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.894	8.91 ng	1069300	Perylene-d12	23.747

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Eicosane	282	C20H42	000112-95-8	95
3	Docosane	310	C22H46	000629-97-0	93
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

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Data File : BM033394.D
Acq On : 10 Dec 2021 15:01
Operator : CG/JU
Sample : M4919-03
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FDR-MW-4-20211202

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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
Phenol, 4-ethen...	15.089	6.9	ng	273634	3	14.530	791466	20.0
2-Piperidinecar...	15.860	3.6	ng	142362	3	14.530	791466	20.0
(E)-2,6-Dimetho...	16.301	6.1	ng	331695	4	17.271	1080750	20.0
Ethanone, 1-(4-...	16.566	2.4	ng	131821	4	17.271	1080750	20.0
(E)-4-(3-Hydrox...	16.660	13.4	ng	721447	4	17.271	1080750	20.0
Syringylacetone	16.813	3.4	ng	180982	4	17.271	1080750	20.0
n-Hexadecanoic ...	18.154	5.4	ng	292759	4	17.271	1080750	20.0
3,5-Dimethoxy-4...	18.442	24.9	ng	1345640	4	17.271	1080750	20.0
trans-Sinapyl a...	18.489	35.4	ng	1912900	4	17.271	1080750	20.0
Pentadecane	18.683	40.7	ng	2201590	4	17.271	1080750	20.0
Octadecanoic ac...	19.424	2.3	ng	135221	5	21.430	1160470	20.0
Heptadecane, 9-...	20.101	43.9	ng	2548720	5	21.430	1160470	20.0
Hexatriacontane	21.077	40.9	ng	2372600	5	21.430	1160470	20.0
Heneicosane	21.883	37.4	ng	2171490	5	21.430	1160470	20.0
13-Tetradecen-1...	21.959	3.7	ng	216598	5	21.430	1160470	20.0
Hexacosane	22.753	16.2	ng	1945080	6	23.747	2399860	20.0
Eicosane	24.894	8.9	ng	1069300	6	23.747	2399860	20.0