LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

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-BM122121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.472	374	380	396	rVB	328448	492752	24.38%	3.682%
2	7.078	647	653	667	rBV	191327	326892	16.17%	2.443%
3	7.907	788	794	801	rBV	105446	172389	8.53%	1.288%
4	9.084	986	994	1009	rBV	467186	820235	40.58%	6.129%
5	10.060	1151	1160	1166	rBV	31765	58056	2.87%	0.434%
6	10.719	1265	1272	1280	rBV	134027	234849	11.62%	1.755%
7	13.177	1683	1690	1701	rBV	1152035	1726964	85.44%	12.904%
8	14.554	1918	1924	1937	rVB	202862	307082	15.19%	2.294%
9	16.048	2171	2178	2193	rBV	934181	1328709	65.73%	9.928%
10	17.054	2343	2349	2354	rBV2	16992	25541	1.26%	0.191%
11	17.301	2386	2391	2399	rBV	246318	360681	17.84%	2.695%
12	17.795	2469	2475	2479	rBV	113561	141269	6.99%	1.056%
13	17.971	2500	2505	2510	rBV	257704	308998	15.29%	2.309%
14	18.489	2587	2593	2598	rBV	268867	341039	16.87%	2.548%
15	19.112	2694	2699	2702	rBV2	1641792	2021332	100.00%	15.103%
16	19.148	2702	2705	2709	rVB2	847072	991668	49.06%	7.410%
17	19.277	2723	2727	2732	rBV	75865	88658	4.39%	0.662%
18	19.354	2737	2740	2746	rVB6	20719	30411	1.50%	0.227%
19	19.489	2756	2763	2767	rBV3	21927	38731	1.92%	0.289%
20	19.695	2794	2798	2803	rBV	199927	223980	11.08%	1.674%
21	19.924	2832	2837	2842	rBV	1658886	2010835	99.48%	15.025%
22	20.230	2885	2889	2892	rBV	85108	93257	4.61%	0.697%
23	20.724	2970	2973	2976	rVB2	31023	34451	1.70%	0.257%
24	21.183	3048	3051	3056	rBV3	46947	61841	3.06%	0.462%
25	21.483	3097	3102	3107	rBV	293002	400168	19.80%	2.990%
26	22.583	3285	3289	3299	rVB	268526	376162	18.61%	2.811%
27	23.877	3503	3509	3516	rVB	186254	366453	18.13%	2.738%

Sum of corrected areas: 13383403

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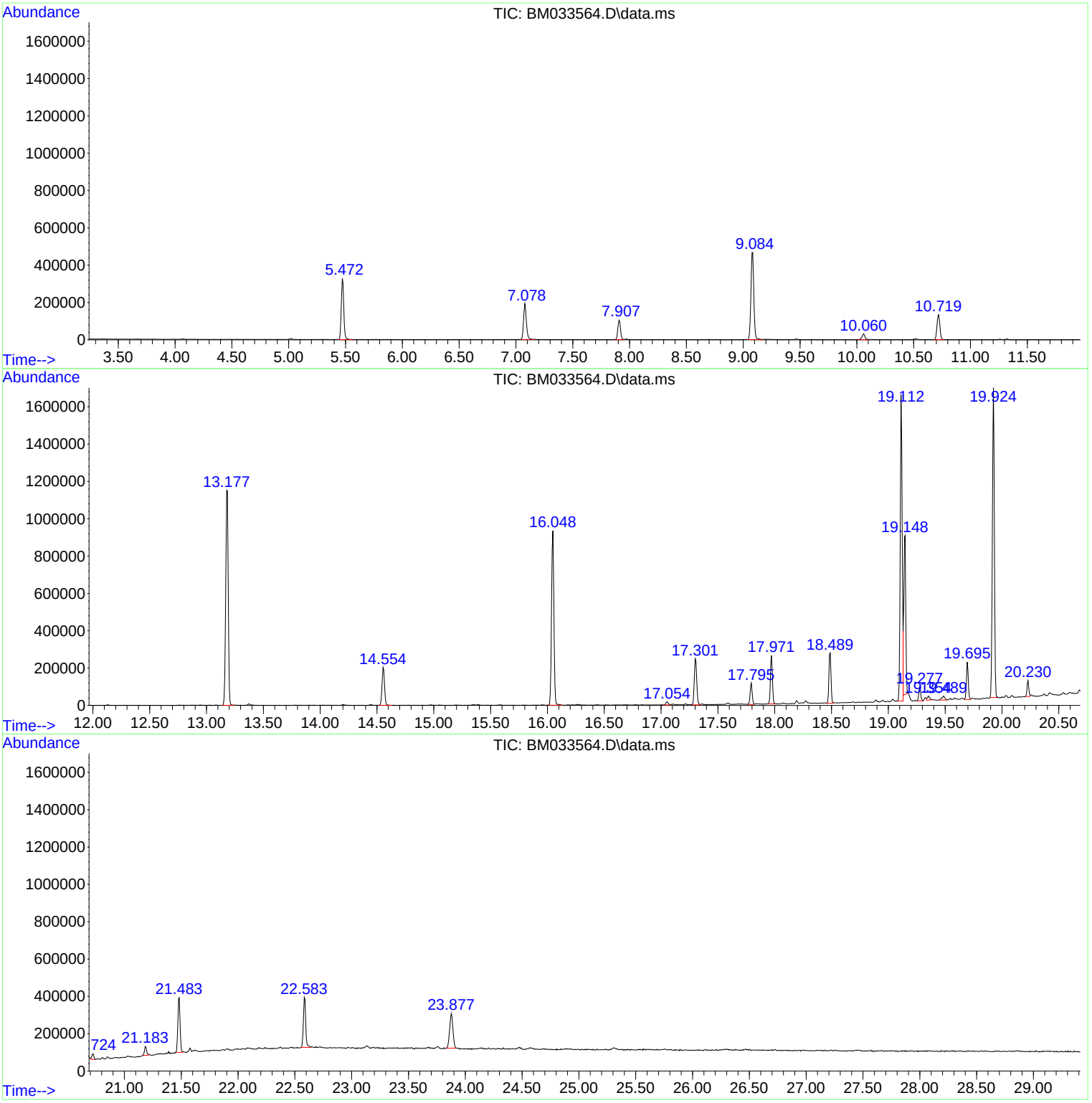
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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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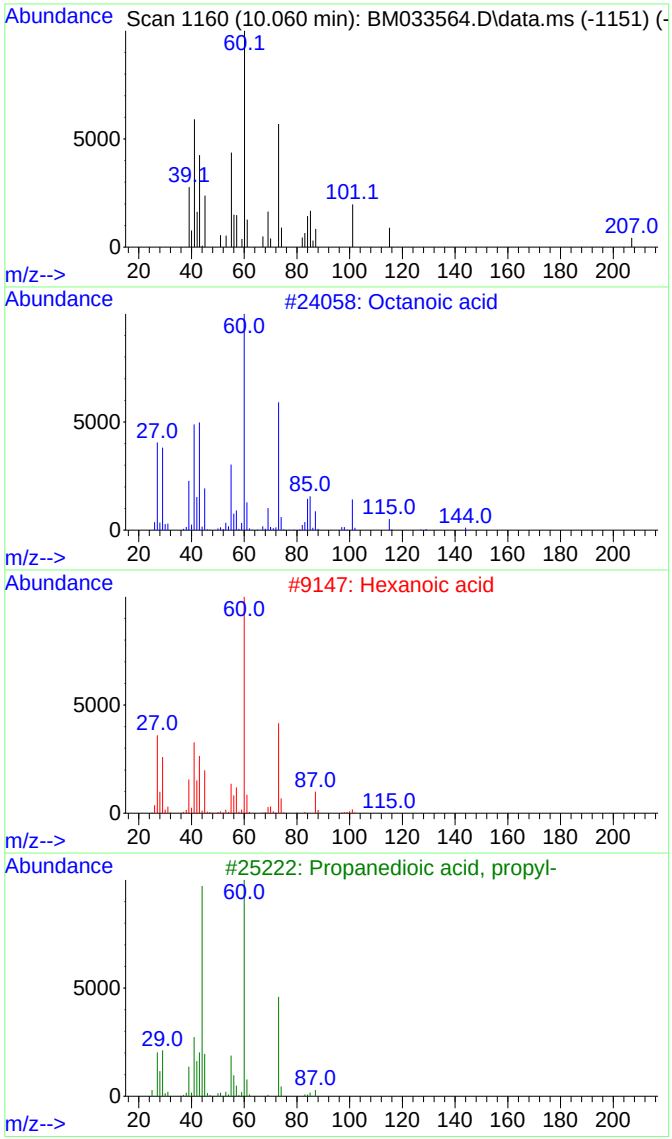
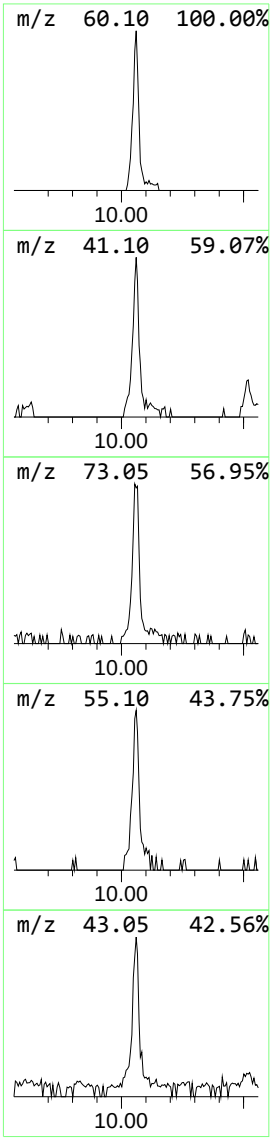
Peak Number 1 Octanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.060	4.94 ng	58056	Naphthalene-d8	10.719

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	86
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	59
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
5	D-Fucose	164	C6H12O5	003615-37-0	53





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Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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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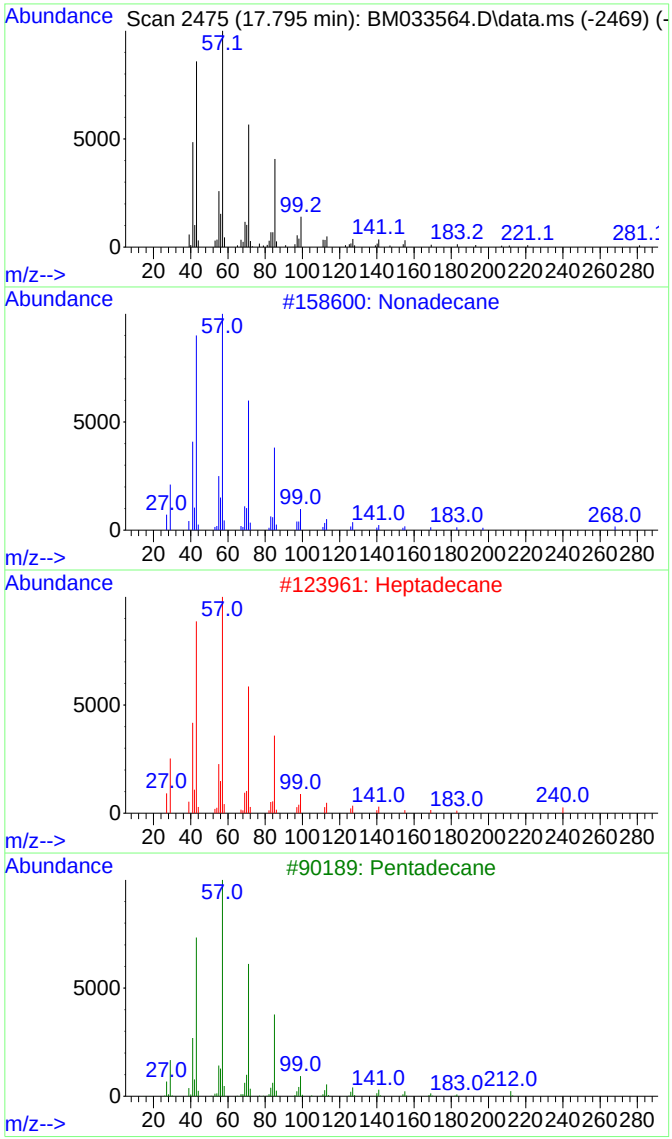
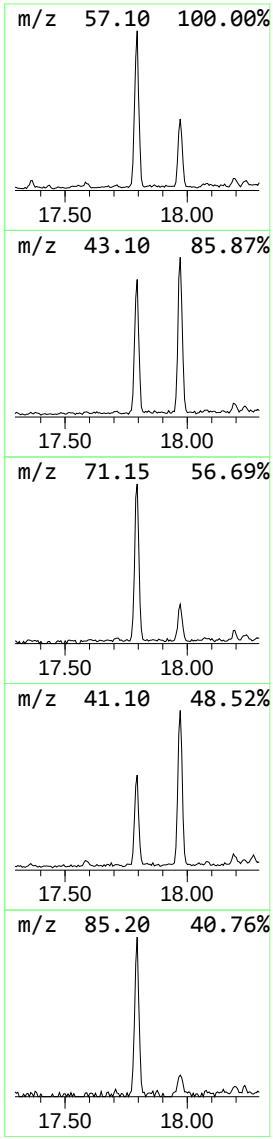
Peak Number 2 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.795	7.83 ng	141269	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Tritetracontane	605	C43H88	007098-21-7	90
5	Tridecane	184	C13H28	000629-50-5	90





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Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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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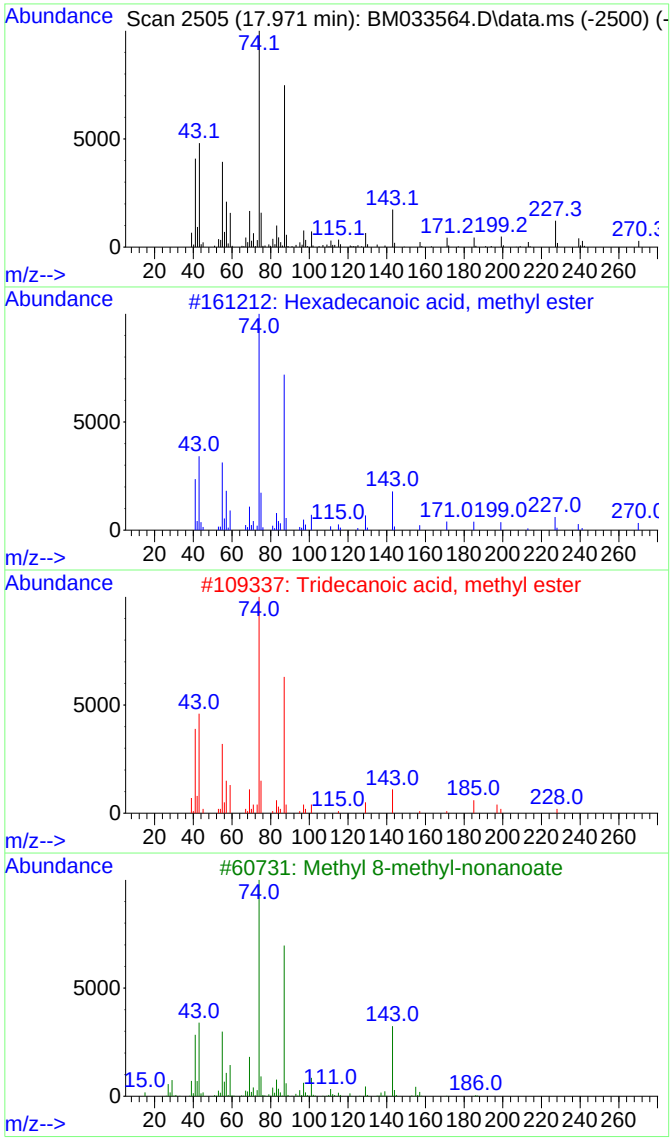
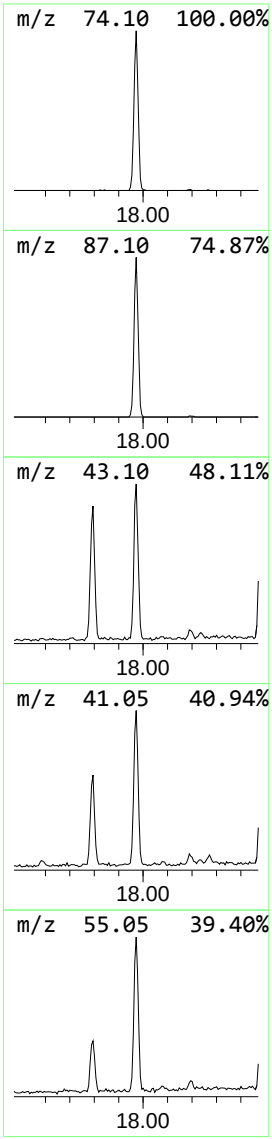
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.971	17.13 ng	308998	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	90
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87





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Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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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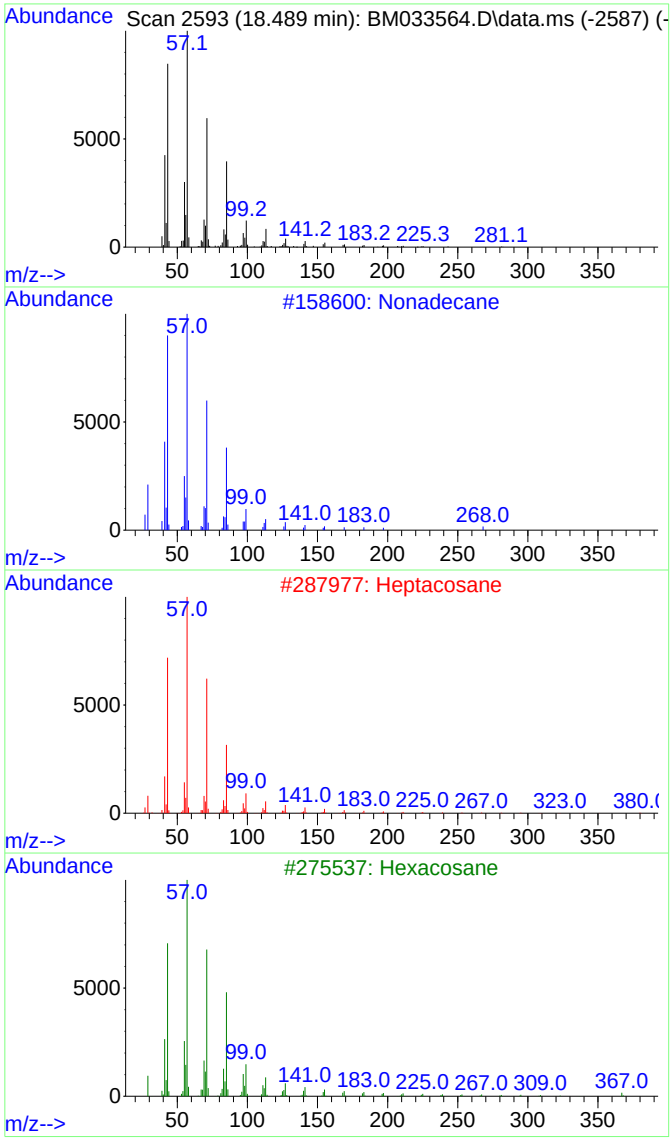
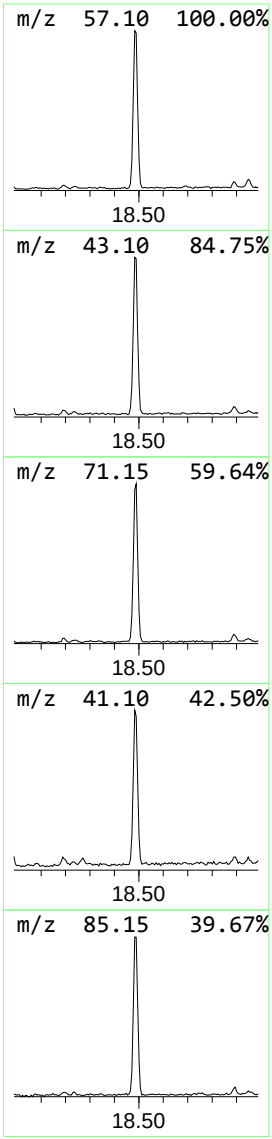
Peak Number 4 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	18.91 ng	341039	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane	310	C22H46	000629-97-0	91
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	91





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Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

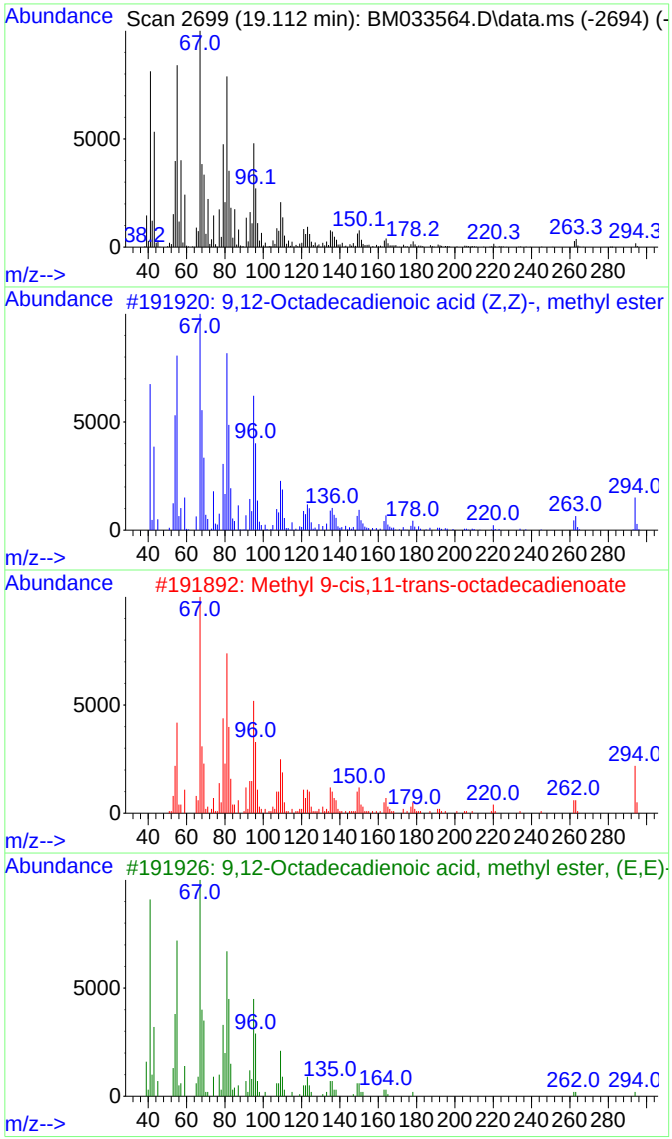
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

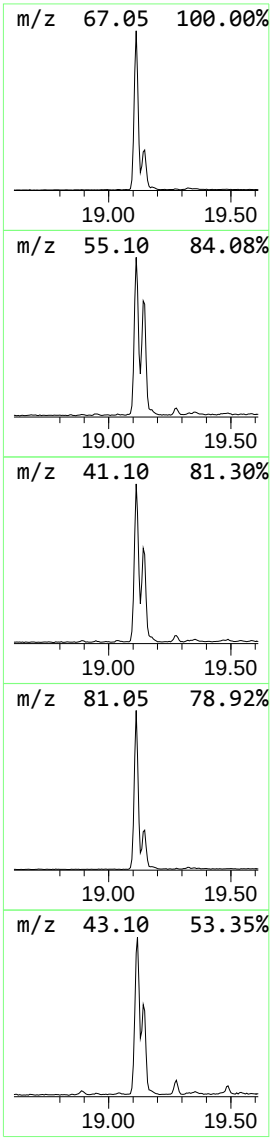
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.112	112.08 ng	2021330	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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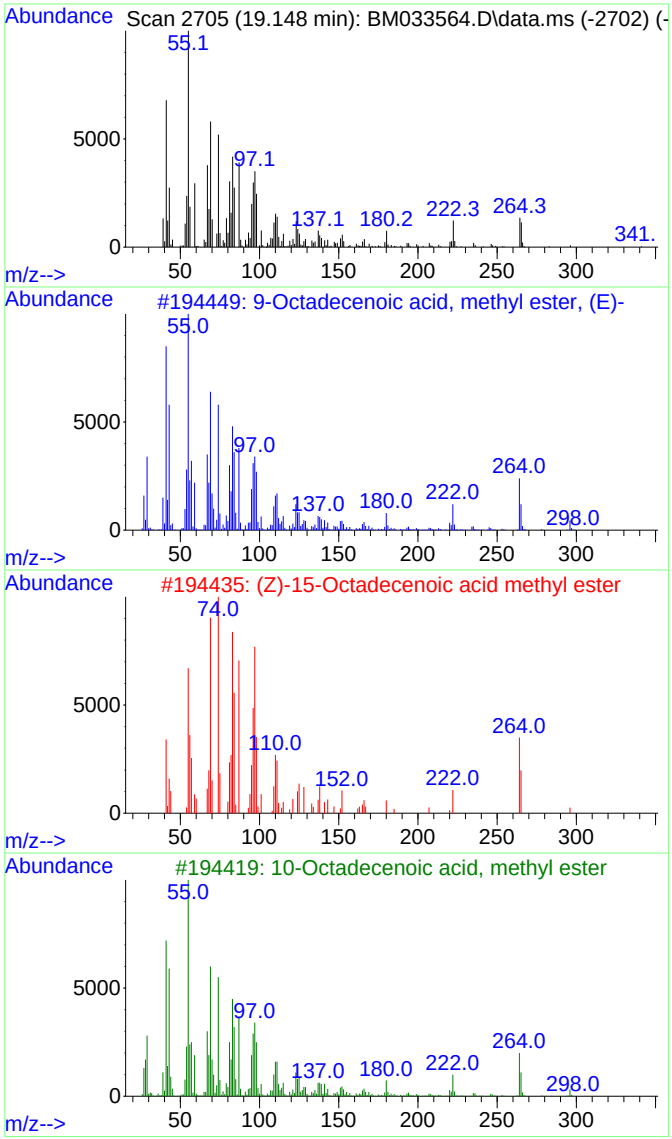
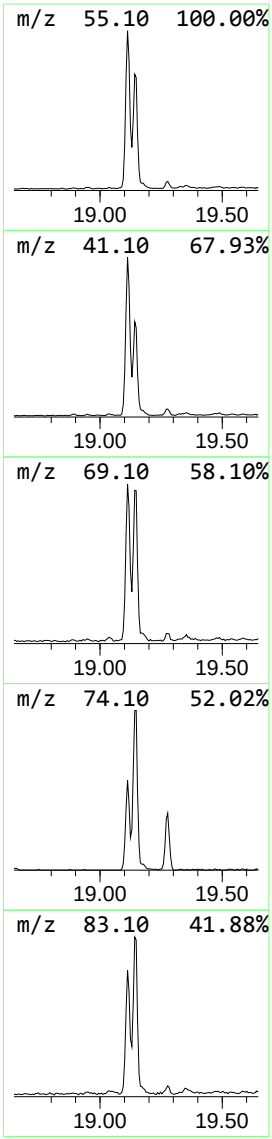
Peak Number 6 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.148	54.99 ng	991668	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	91





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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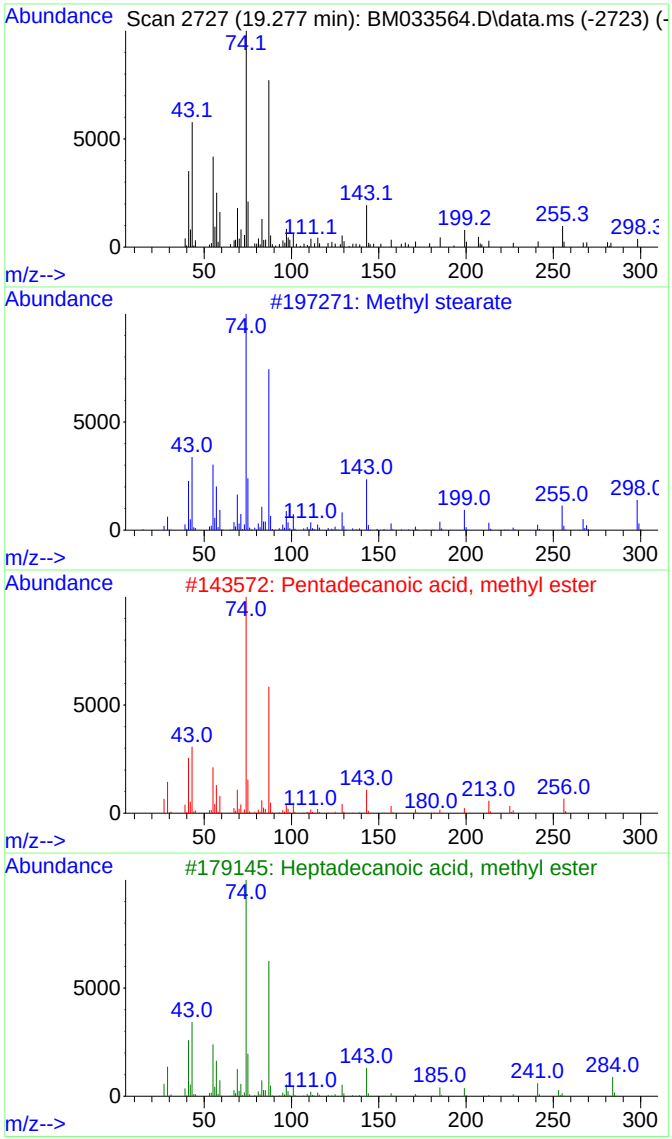
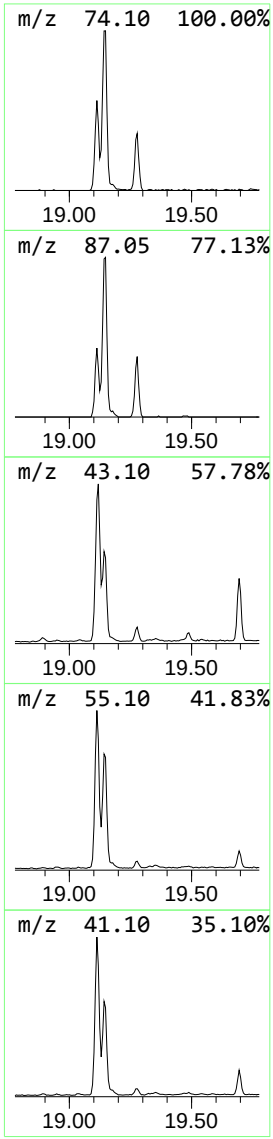
Peak Number 7 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.277	4.92 ng	88658	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5	2-Methylpentadecanoic acid	256	C16H32O2	025354-92-1	76





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
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TIC Library : C:\Database\NIST20.L
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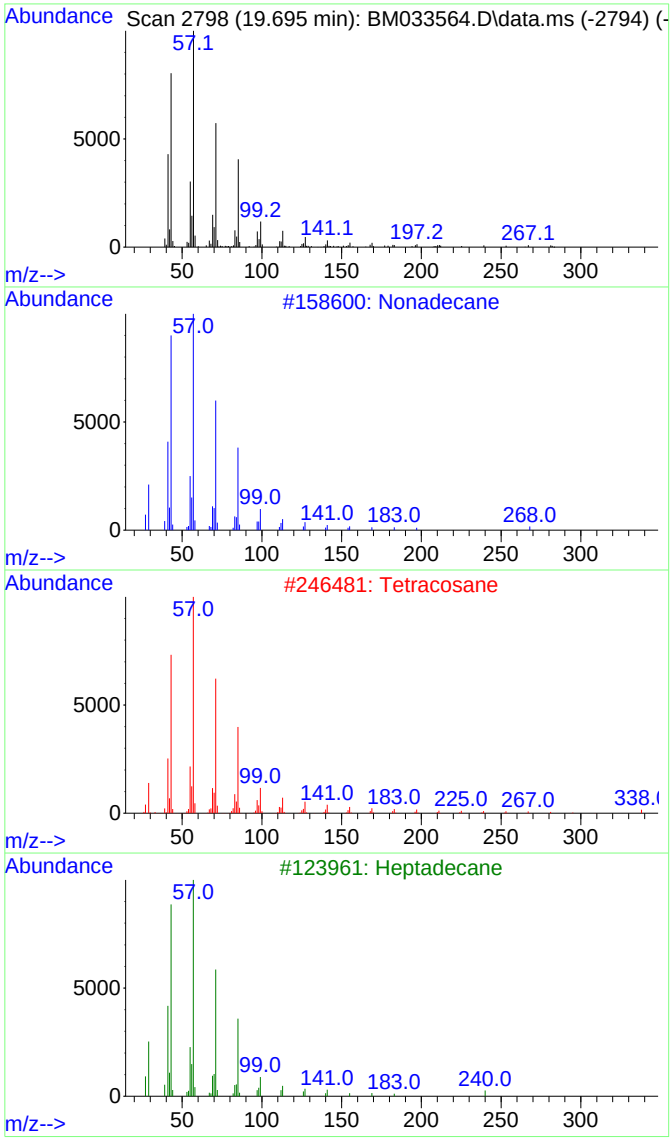
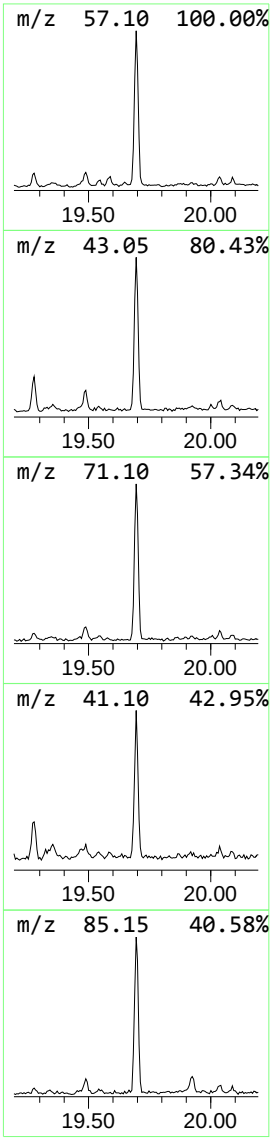
Peak Number 8 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.695	11.19 ng	223980	Chrysene-d12	21.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	91
5	Pentadecane	212	C15H32	000629-62-9	91





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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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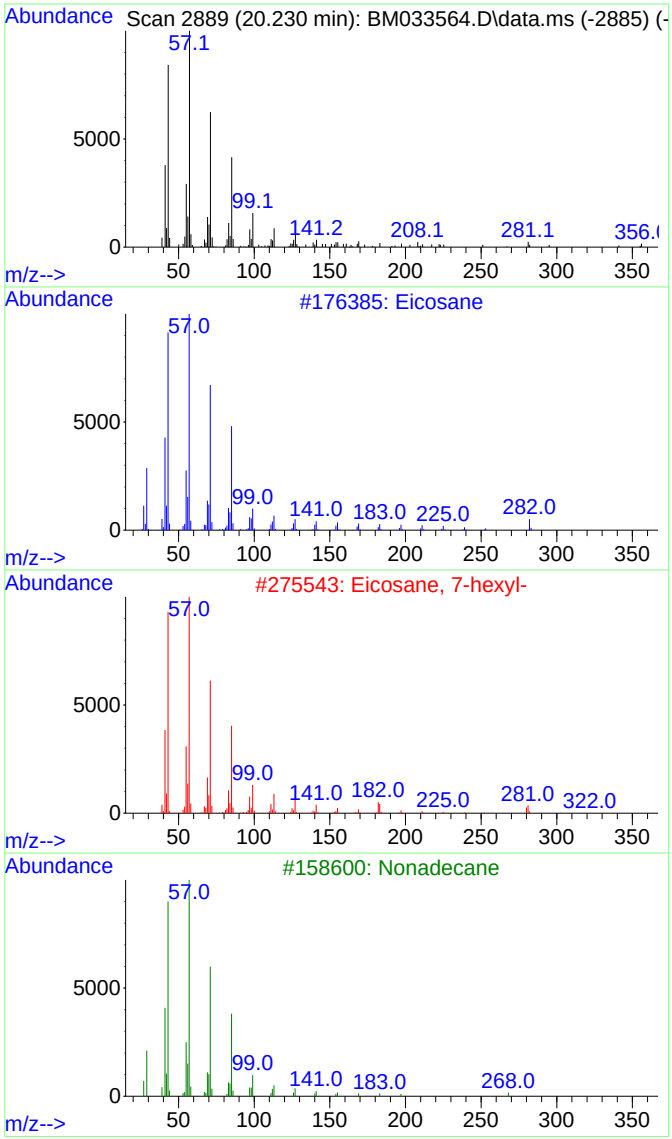
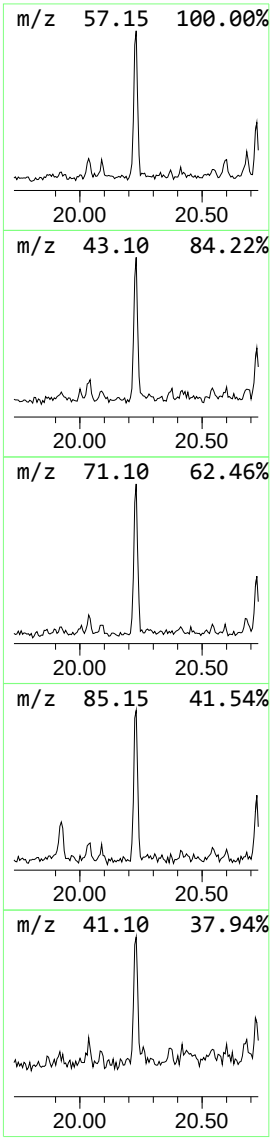
Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.230	4.66 ng	93257	Chrysene-d12	21.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





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Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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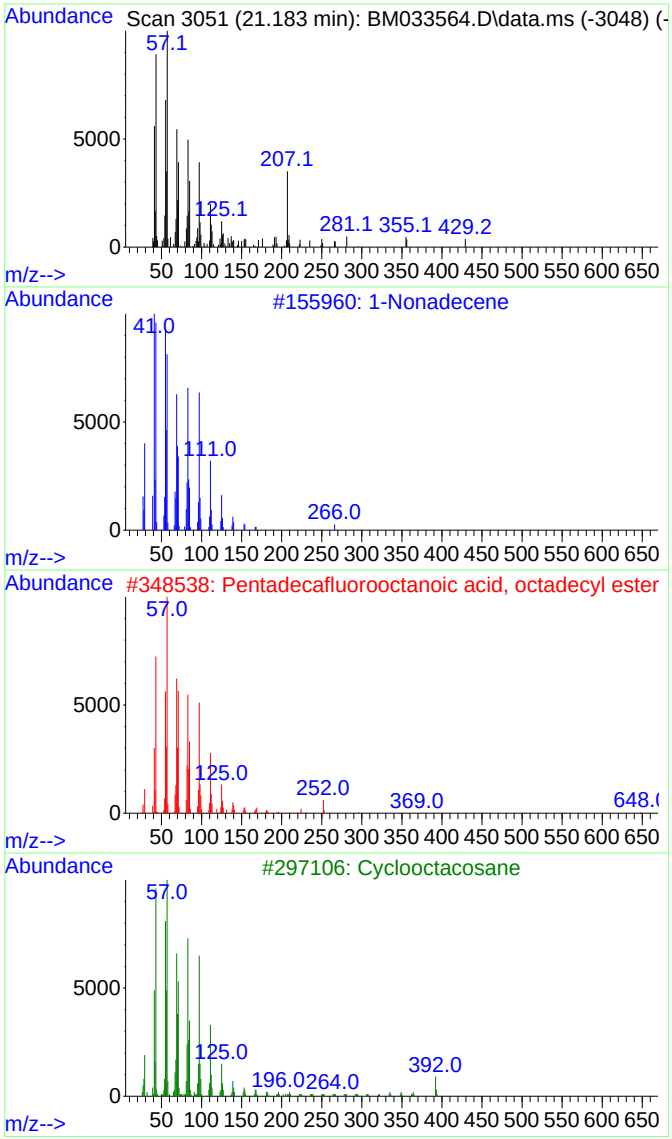
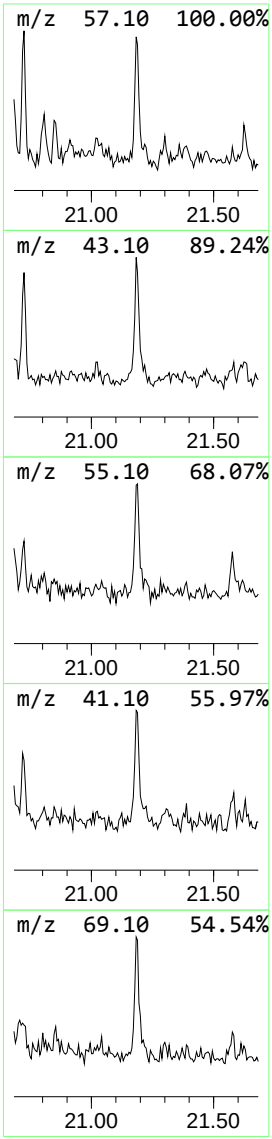
Peak Number 10 1-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.183	3.09 ng	61841	Chrysene-d12	21.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	83
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81
3	Cyclooctacosane	392	C28H56	000297-24-5	81
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

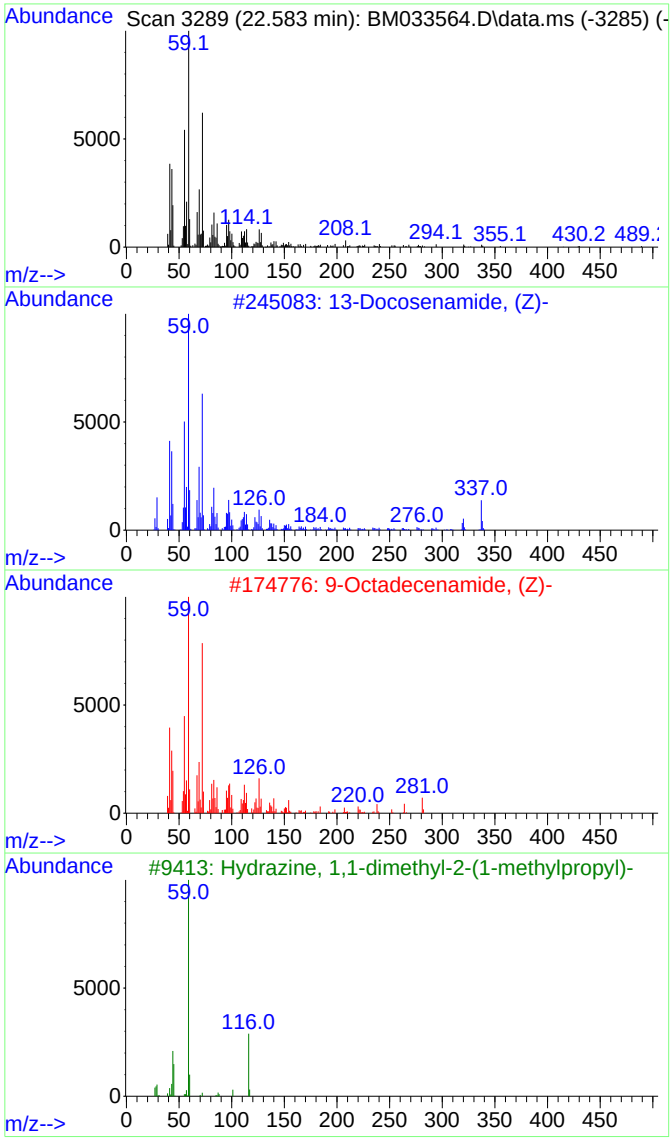
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

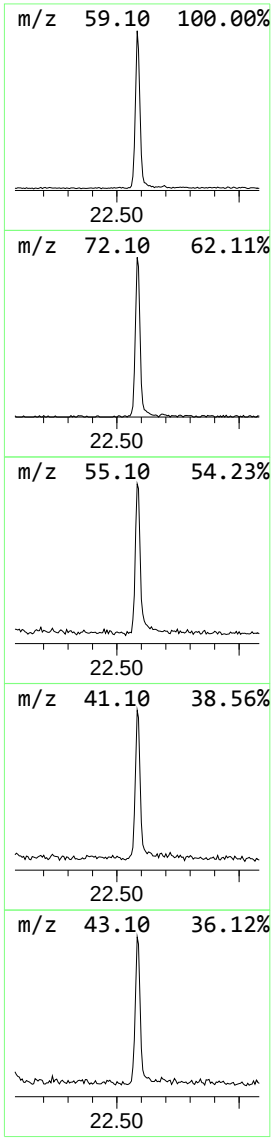
****

Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.583	18.80 ng	376162	Chrysene-d12	21.483

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Hydrazine, 1,1-dimethyl-2-(1-met...	116	C6H16N2	054007-24-8	49
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	38
5	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122121\
Data File : BM033564.D
Acq On : 21 Dec 2021 21:14
Operator : CG/JU
Sample : M5182-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EQUIPMENT-BLANK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM122121.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
Octanoic acid	10.060	4.9	ng	58056	2	10.719	234849	20.0
Nonadecane	17.795	7.8	ng	141269	4	17.301	360681	20.0
Hexadecanoic ac...	17.971	17.1	ng	308998	4	17.301	360681	20.0
Heptacosane	18.489	18.9	ng	341039	4	17.301	360681	20.0
9,12-Octadecadi...	19.112	112.1	ng	2021330	4	17.301	360681	20.0
9-Octadecenoic ...	19.148	55.0	ng	991668	4	17.301	360681	20.0
Methyl stearate	19.277	4.9	ng	88658	4	17.301	360681	20.0
Tetracosane	19.695	11.2	ng	223980	5	21.483	400168	20.0
Eicosane	20.230	4.7	ng	93257	5	21.483	400168	20.0
1-Nonadecene	21.183	3.1	ng	61841	5	21.483	400168	20.0
13-Docosenamide...	22.583	18.8	ng	376162	5	21.483	400168	20.0