LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047281.D
Acq On : 20 Aug 2024 22:14
Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	61	64	75	rBV	141088	216552	1.49%	0.293%
2	4.569	278	286	296	rVB2	92472	147476	1.01%	0.199%
3	5.016	355	362	377	rBV	2932136	4311838	29.60%	5.824%
4	6.569	620	626	641	rBV	1826763	2956970	20.30%	3.994%
5	7.357	753	760	767	rBV	1122526	1732600	11.89%	2.340%
6	8.504	947	955	965	rBV	2932468	4871951	33.45%	6.581%
7	10.110	1221	1228	1236	rBV	1374704	2272506	15.60%	3.070%
8	10.875	1350	1358	1368	rBV	165280	333563	2.29%	0.451%
9	12.251	1586	1592	1602	rBV	133712	209556	1.44%	0.283%
10	12.628	1648	1656	1665	rBV	7180259	10933668	75.06%	14.769%
11	14.016	1886	1892	1900	rBV	2133858	3056263	20.98%	4.128%
12	15.527	2142	2149	2160	rBV	6064428	8783255	60.30%	11.864%
13	15.780	2188	2192	2200	rVB	101664	156492	1.07%	0.211%
14	16.574	2322	2327	2331	rBV	324990	392445	2.69%	0.530%
15	16.627	2331	2336	2348	rVB	114883	199709	1.37%	0.270%
16	16.780	2356	2362	2368	rBV	2510843	3510475	24.10%	4.742%
17	17.316	2448	2453	2458	rBV	543993	637755	4.38%	0.861%
18	17.492	2479	2483	2489	rVB	320739	385896	2.65%	0.521%
19	17.721	2517	2522	2526	rBV	909280	1243375	8.54%	1.680%
20	18.010	2567	2571	2575	rBV	665872	771979	5.30%	1.043%
21	18.657	2675	2681	2683	rBV2	730555	1194600	8.20%	1.614%
22	18.680	2683	2685	2689	rVB3	493762	495360	3.40%	0.669%
23	18.821	2705	2709	2714	rBV	283834	352773	2.42%	0.477%
24	18.892	2718	2721	2730	rVB4	143488	252833	1.74%	0.342%
25	19.015	2738	2742	2751	rBV	325660	514790	3.53%	0.695%
26	19.245	2778	2781	2790	rVB	470313	566714	3.89%	0.766%
27	19.451	2810	2816	2821	rBV	12063607	14566980	100.00%	19.677%
28	19.786	2870	2873	2878	rVB	327195	368935	2.53%	0.498%
29	20.292	2955	2959	2963	rBV	214798	241552	1.66%	0.326%
30	20.757	3034	3038	3052	rVB	816639	1181200	8.11%	1.596%
31	21.021	3077	3083	3089	rBV	2492275	3532081	24.25%	4.771%
32	22.056	3255	3259	3266	rVB2	186420	268442	1.84%	0.363%
33	23.715	3533	3541	3558	rVB	1393071	3369799	23.13%	4.552%

Sum of corrected areas: 74030383

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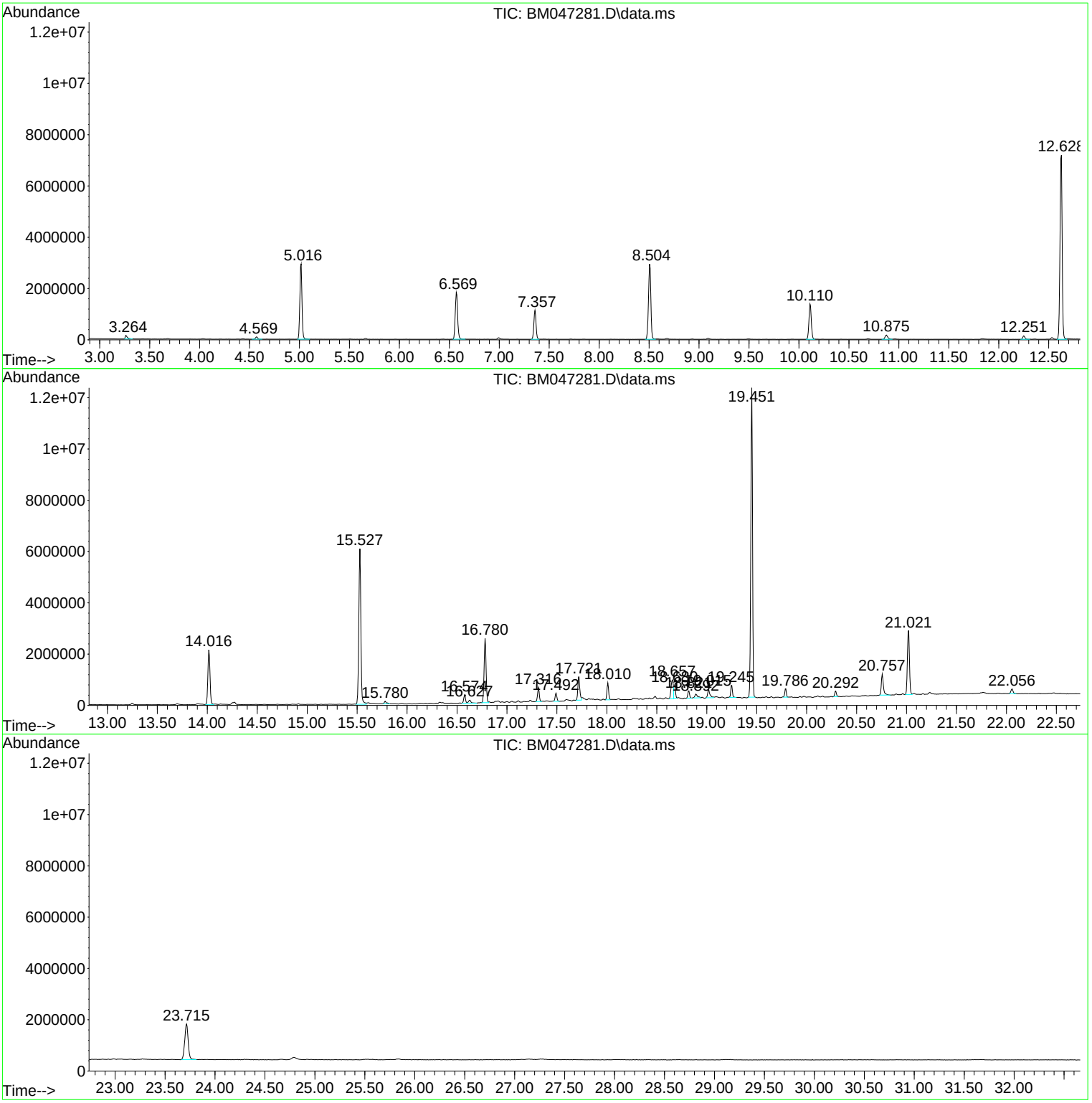
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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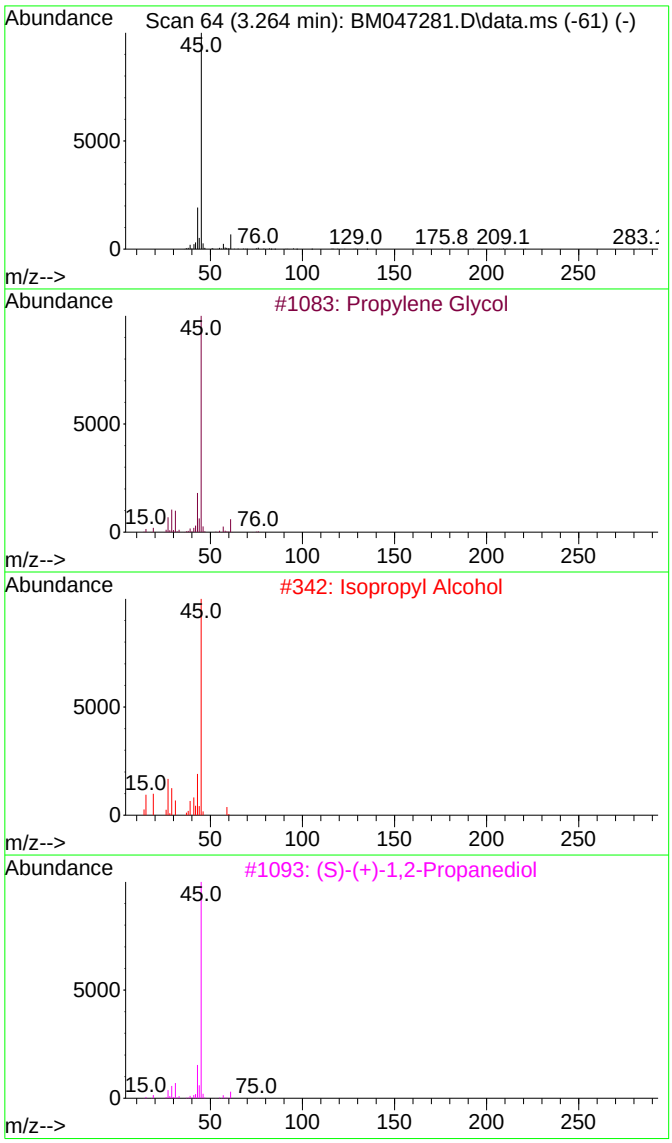
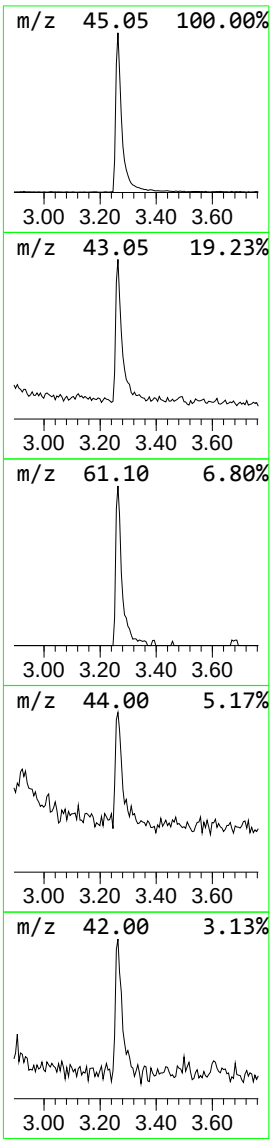
Peak Number 1 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.264	2.50 ng	216552	1,4-Dichlorobenzene-d4	7.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40





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Operator : RC/JU
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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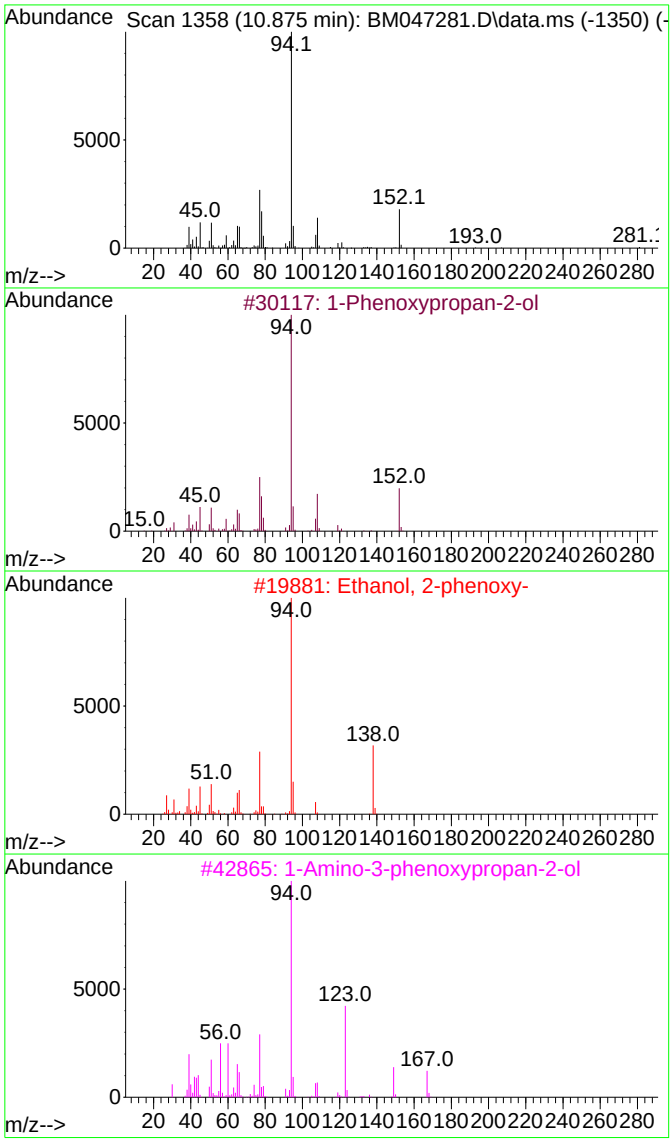
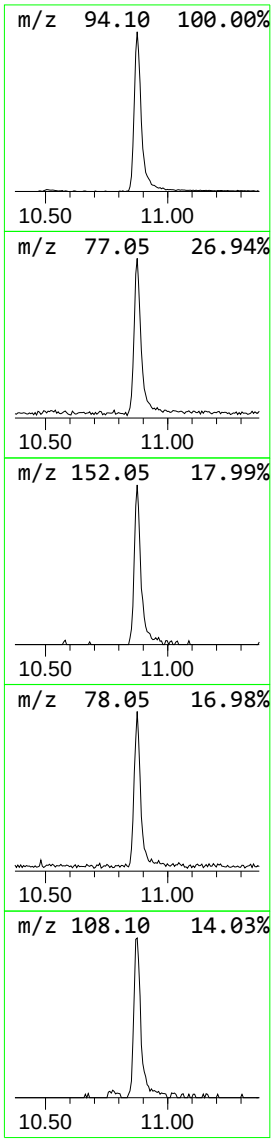
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.94 ng	333563	Naphthalene-d8	10.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3	1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	64
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	60
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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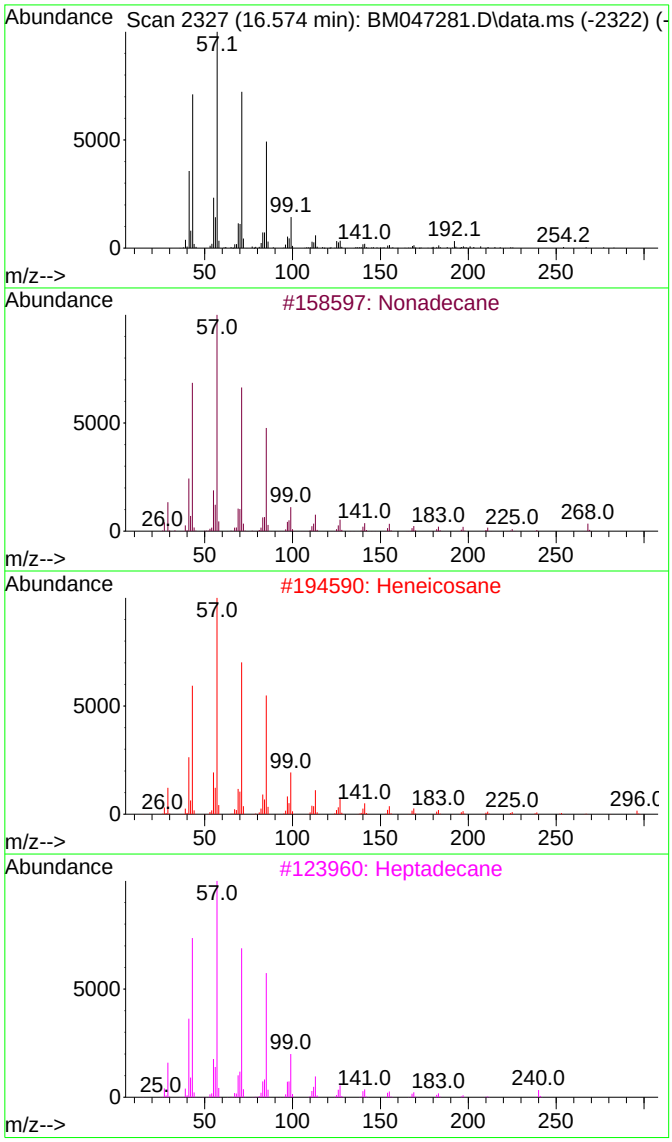
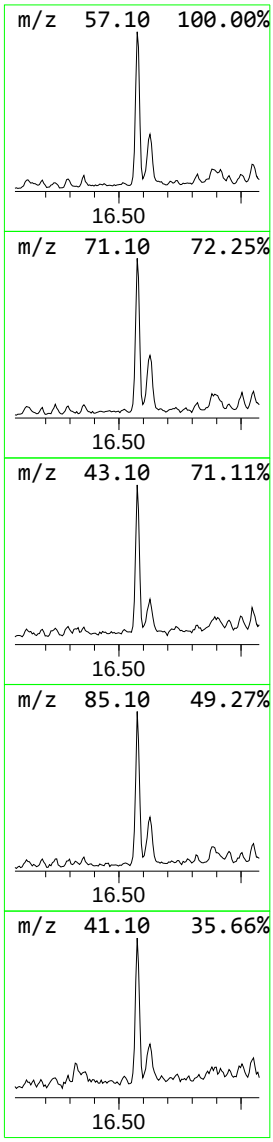
Peak Number 3 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.574	2.24 ng	392445	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Decane, 5-propyl-	184	C13H28	017312-62-8	87
5	Pentadecane	212	C15H32	000629-62-9	86





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Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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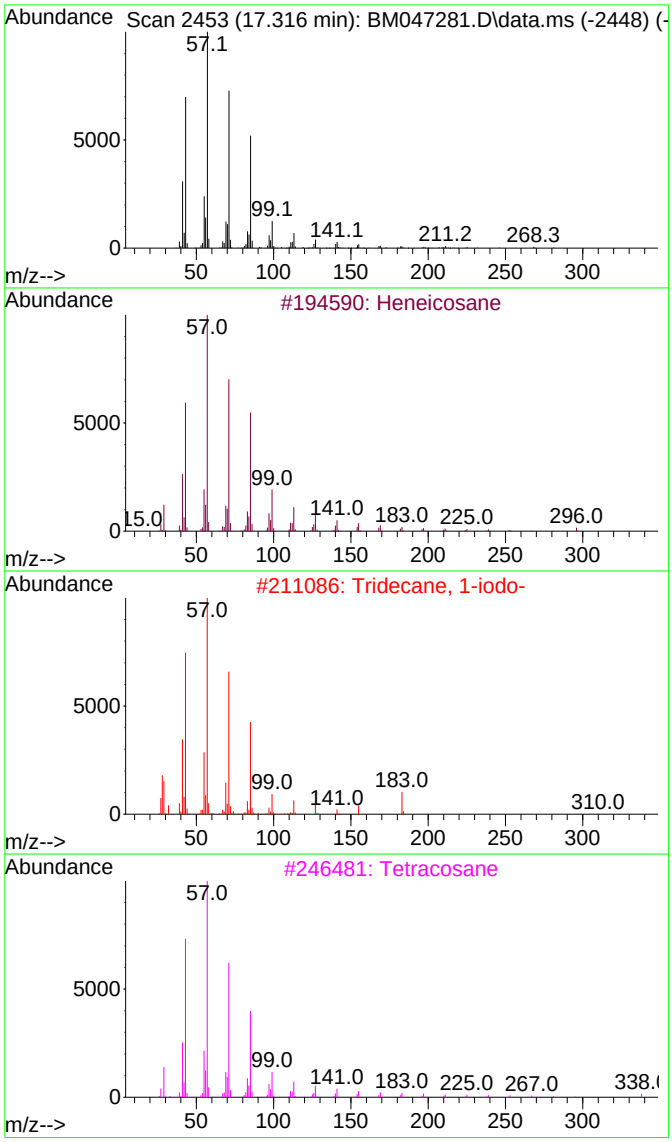
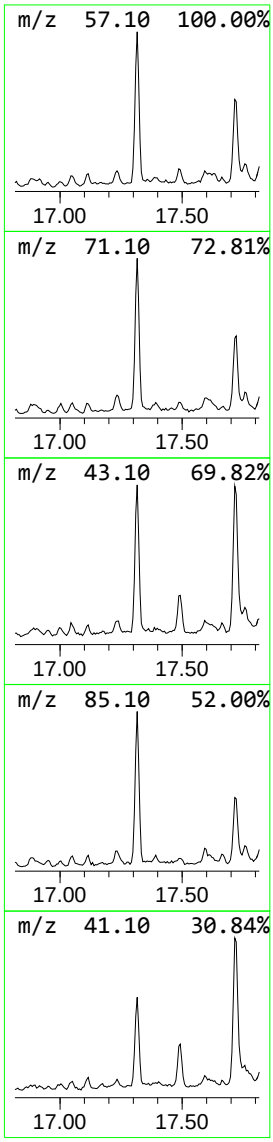
Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.316	3.63 ng	637755	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Decane, 1-iodo-	268	C10H21I	002050-77-3	87
5	9-methylheptadecane	254	C18H38	026741-18-4	86





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Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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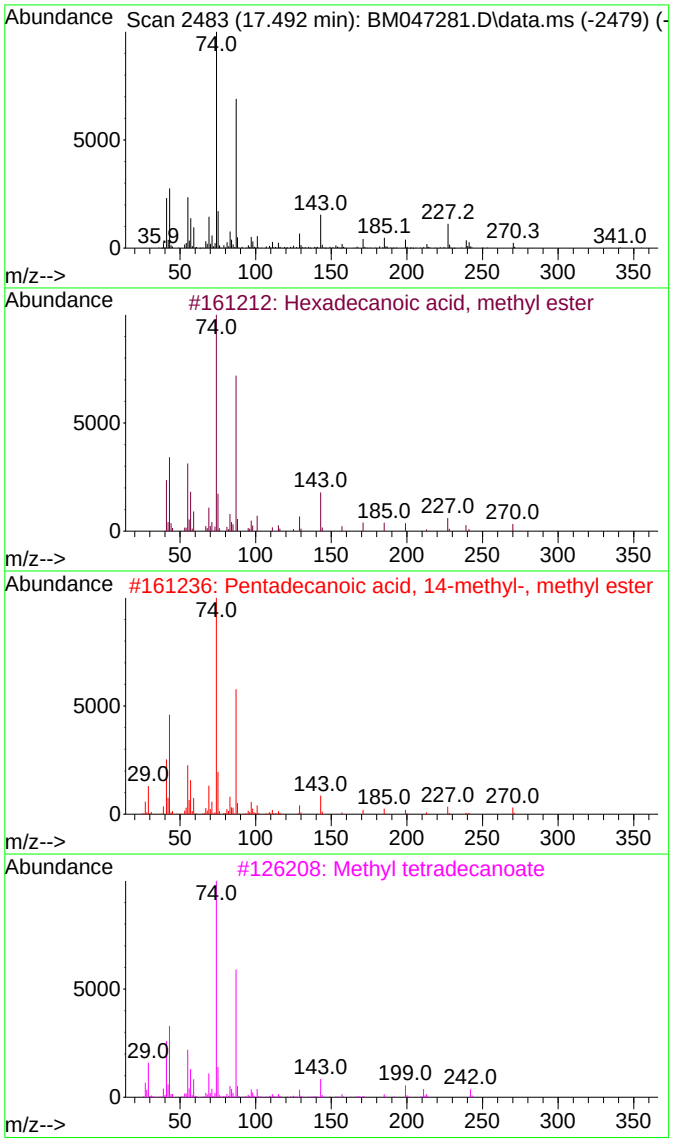
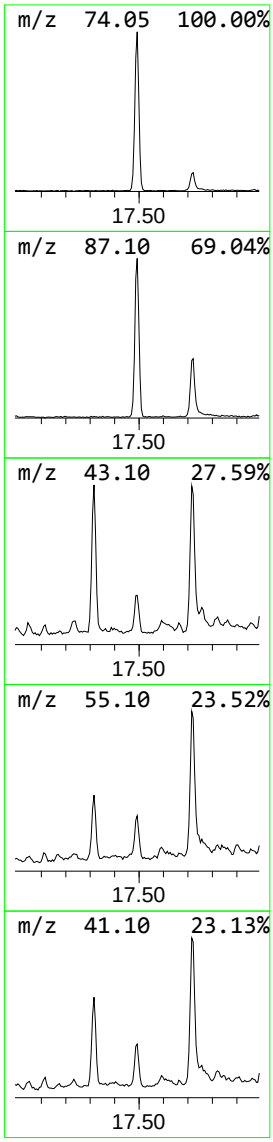
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.492	2.20 ng	385896	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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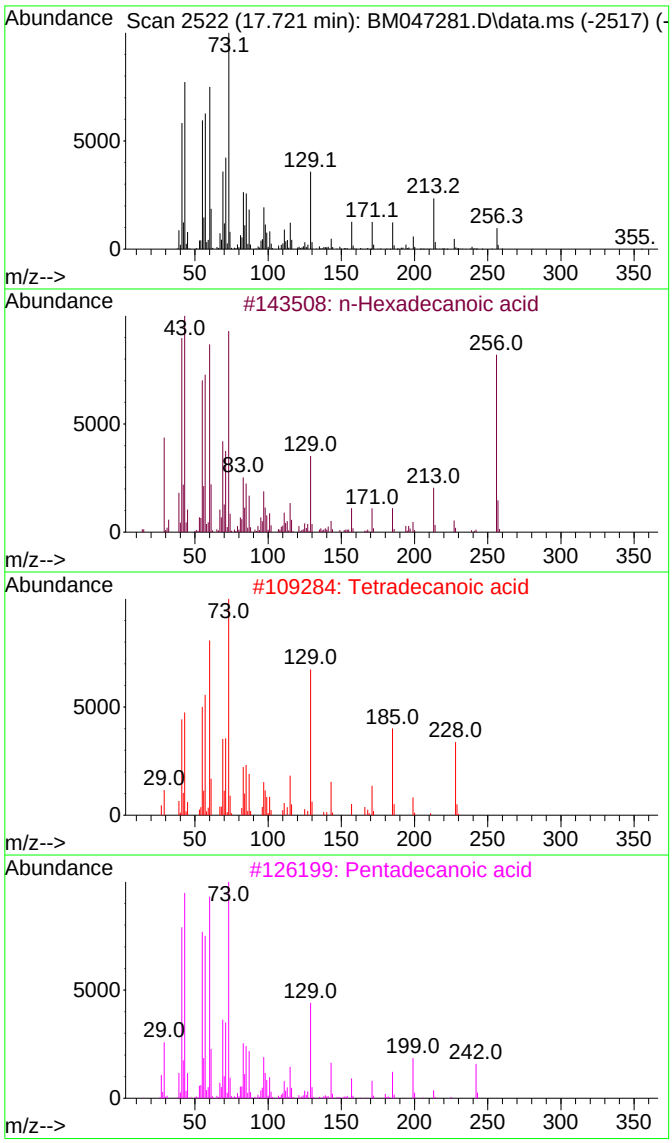
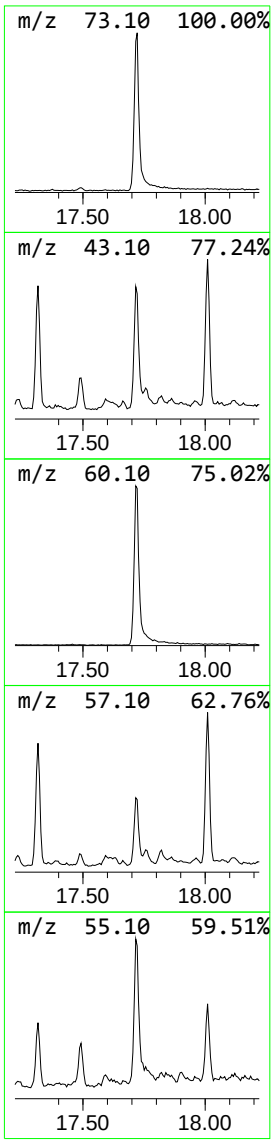
Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	7.08 ng	1243380	Phenanthrene-d10	16.780

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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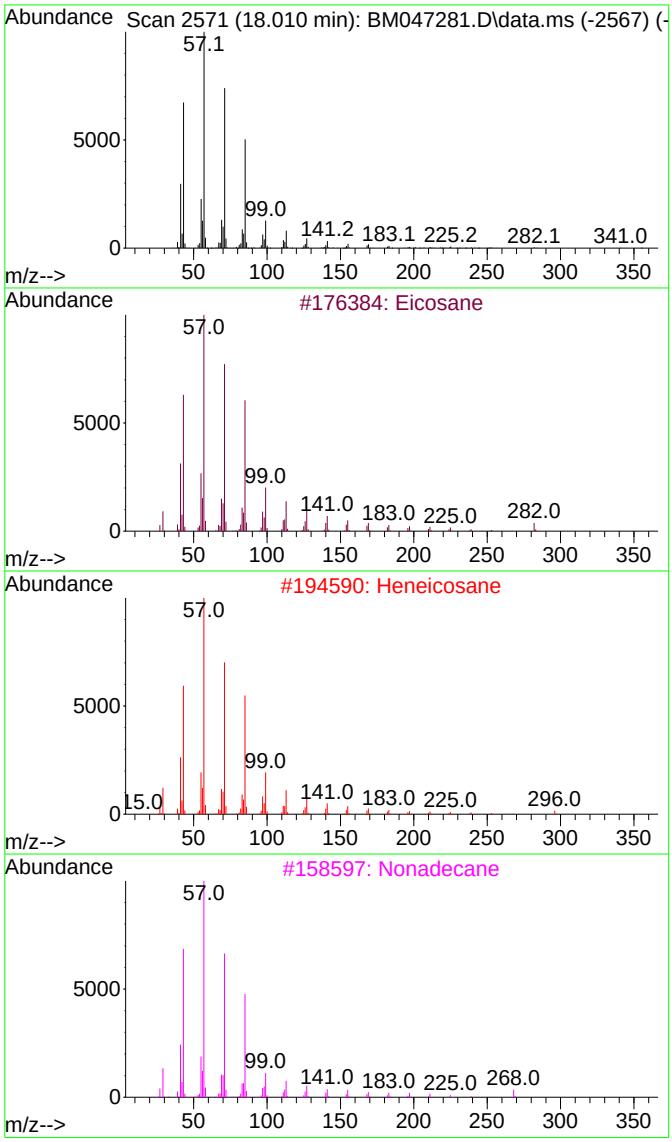
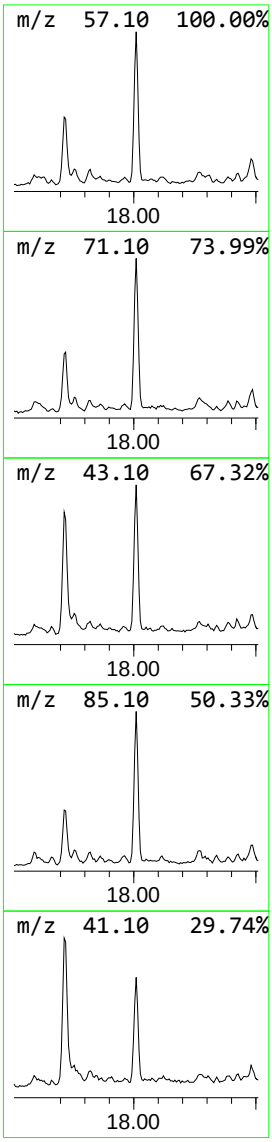
Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	4.40 ng	771979	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87





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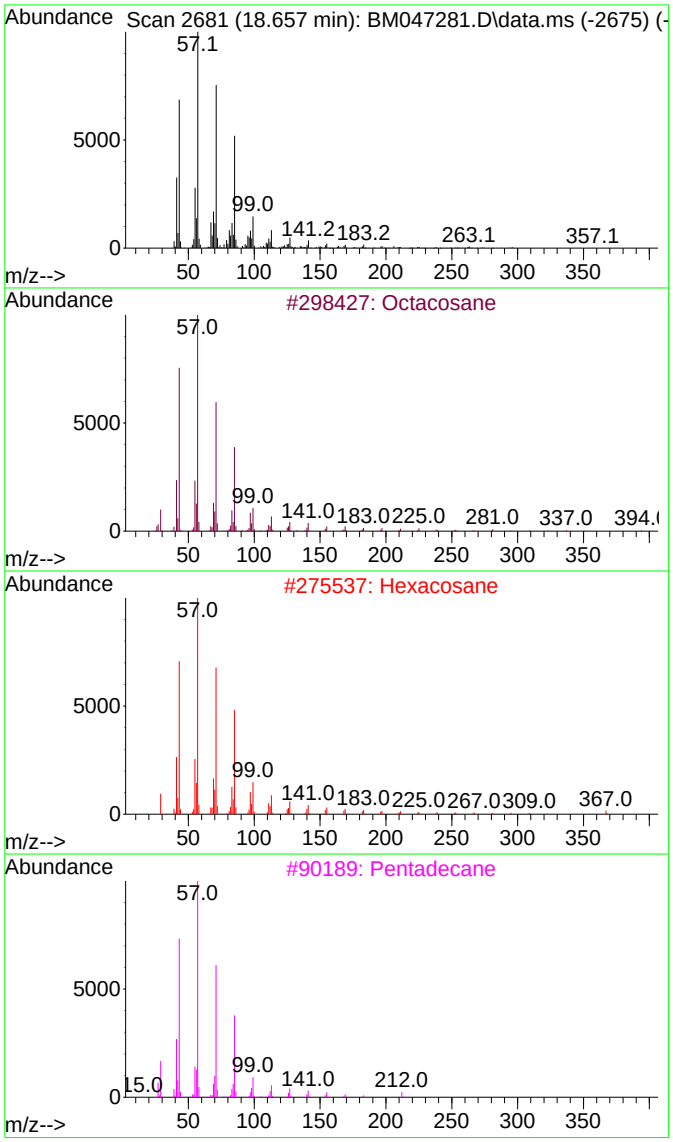
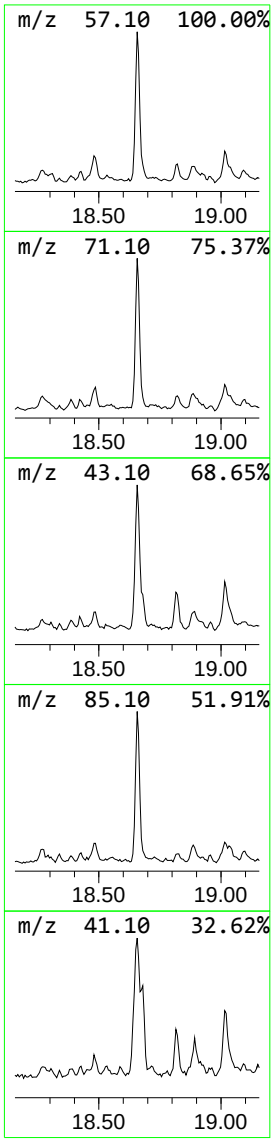
Peak Number 8 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.657	6.81 ng	1194600	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Nonadecane	268	C19H40	000629-92-5	90
5	Tetradecane	198	C14H30	000629-59-4	87





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Instrument :
BNA_M
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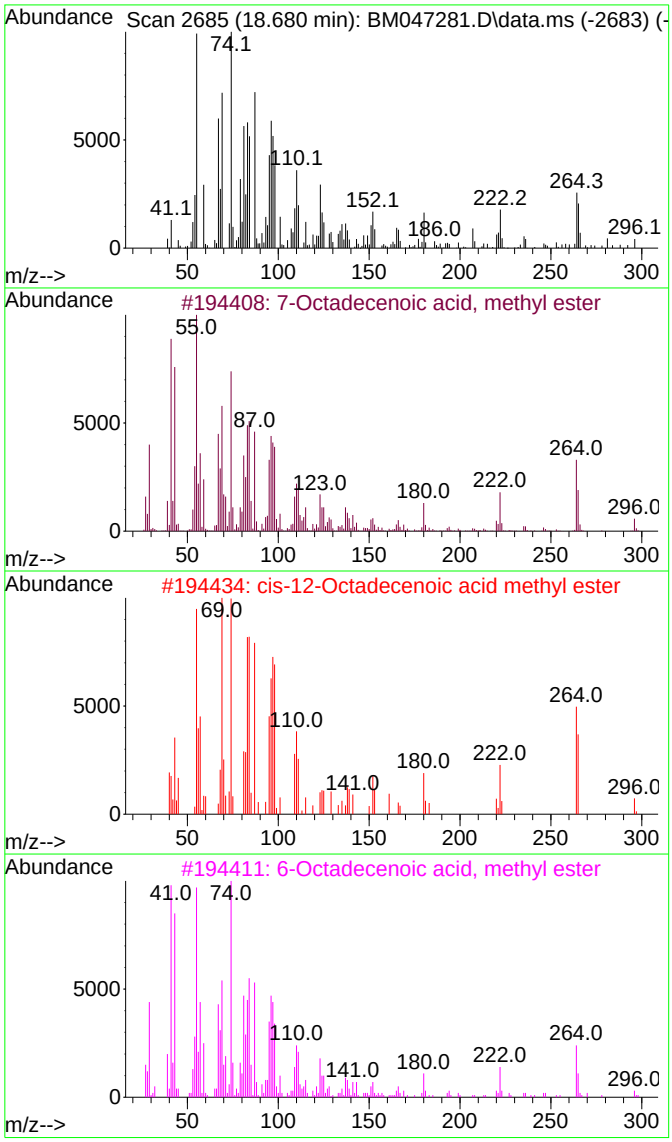
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

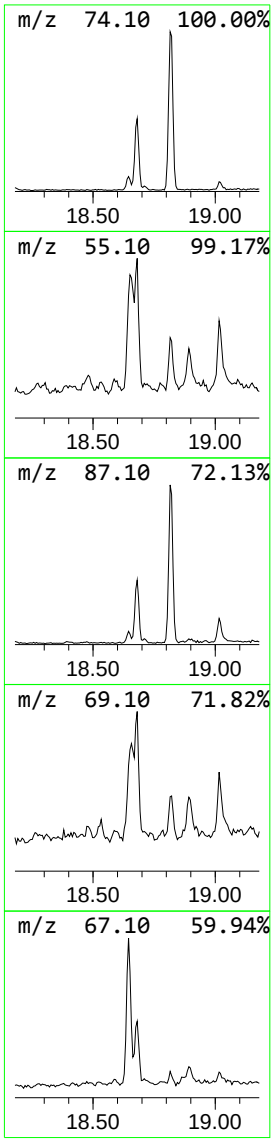
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 7-Octadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.680	2.82 ng	495360	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	98
2	cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	98
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	96
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	96
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94





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ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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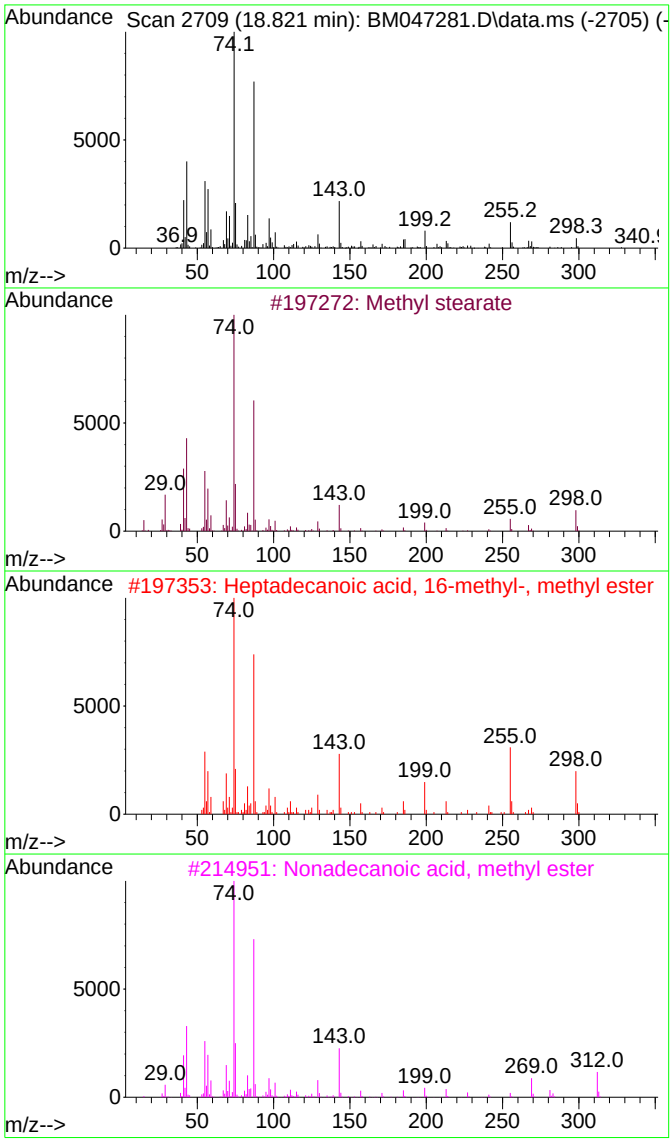
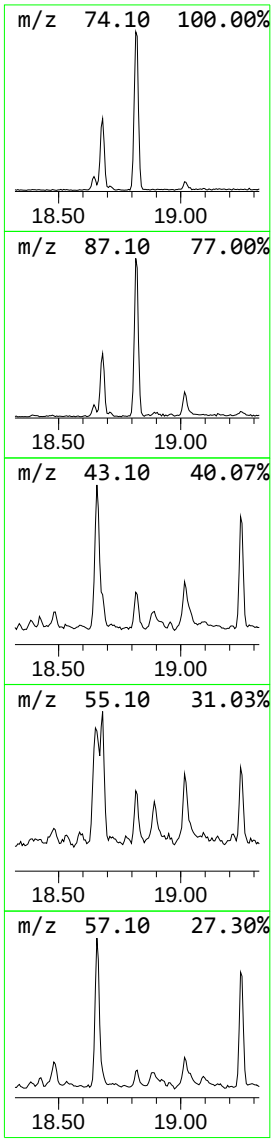
Peak Number 10 Methyl stearate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.821	2.01 ng	352773	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	062691-05-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047281.D
Acq On : 20 Aug 2024 22:14
Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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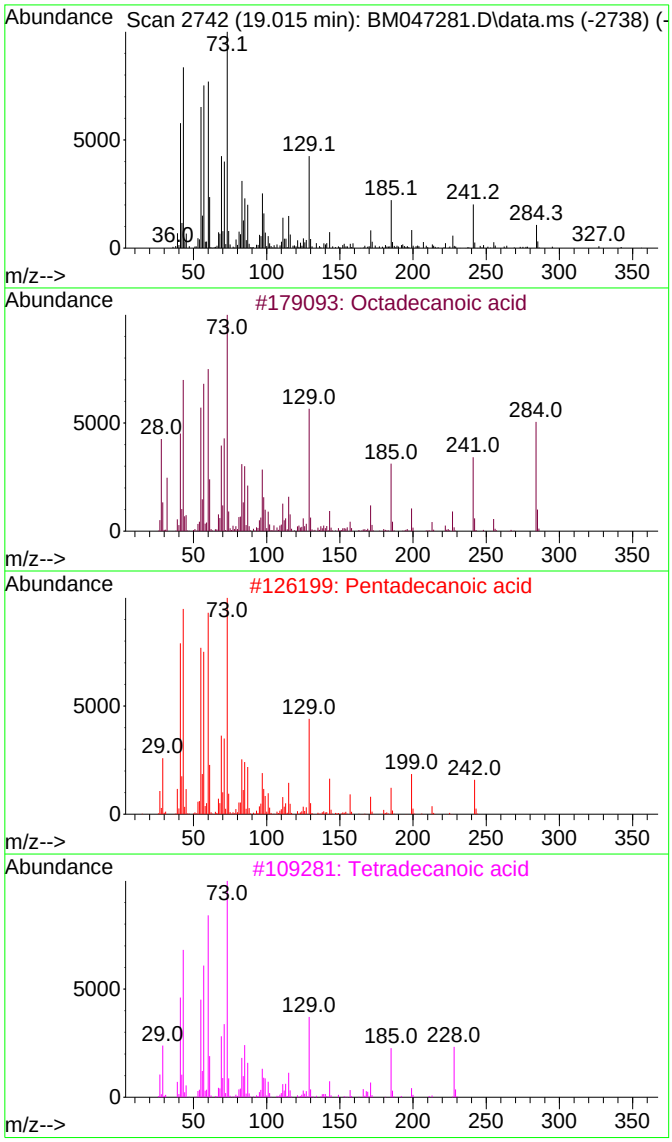
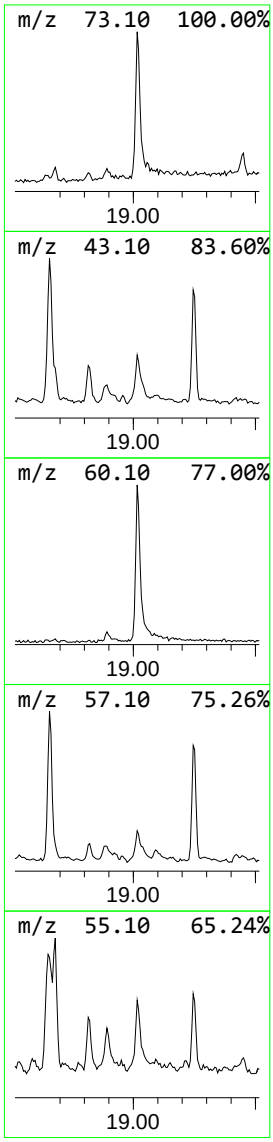
Peak Number 11 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	2.91 ng	514790	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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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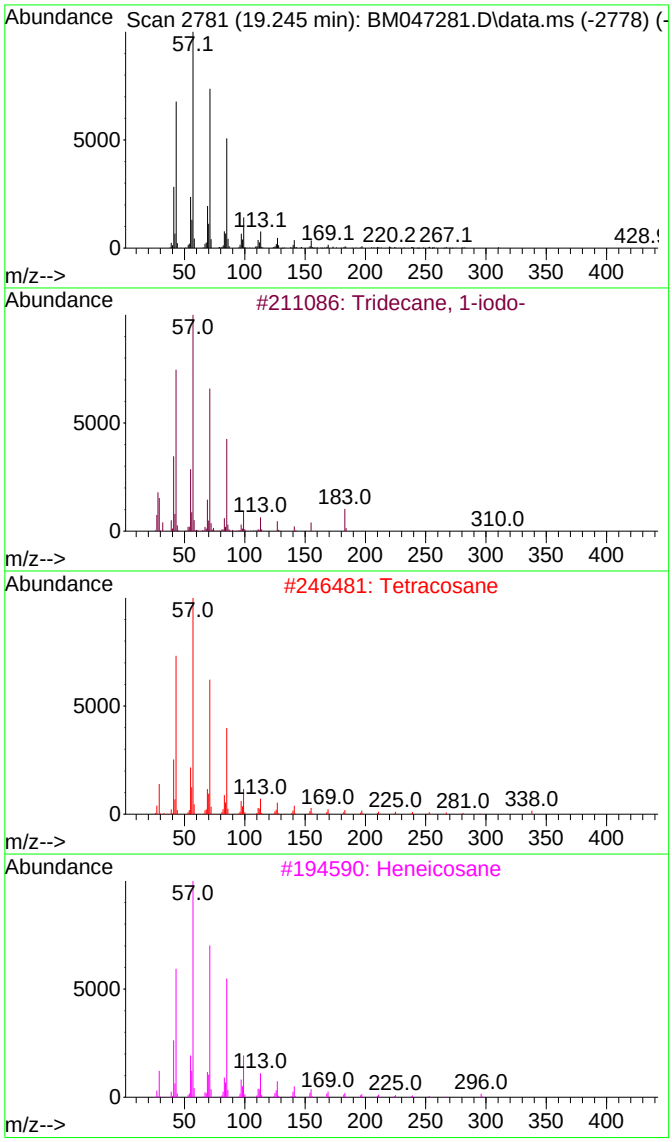
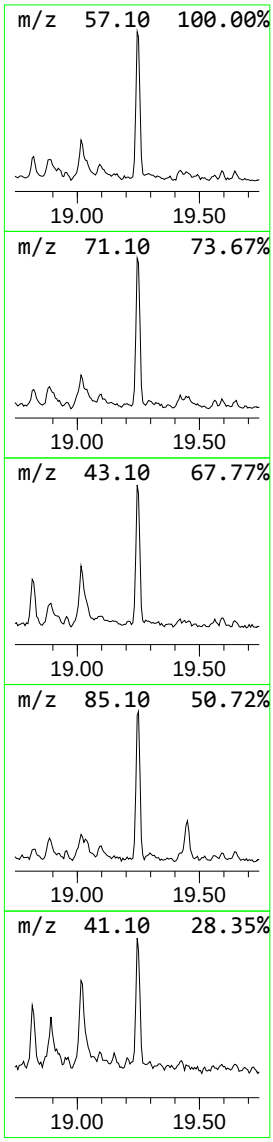
Peak Number 12 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	3.21 ng	566714	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	94
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91





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Data File : BM047281.D
Acq On : 20 Aug 2024 22:14
Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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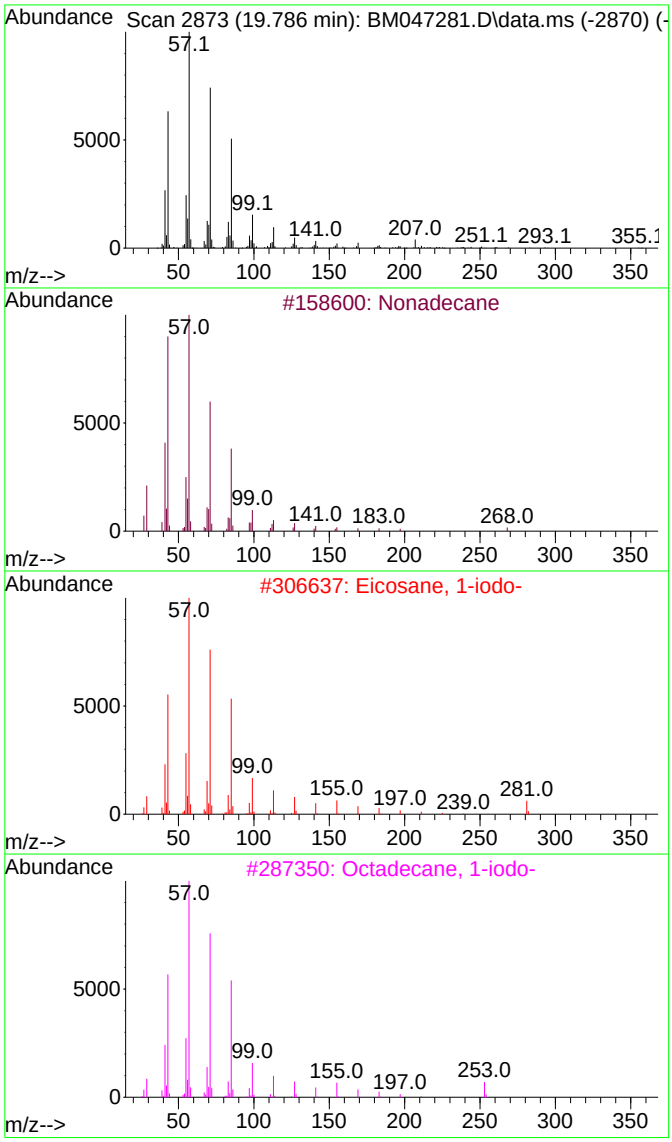
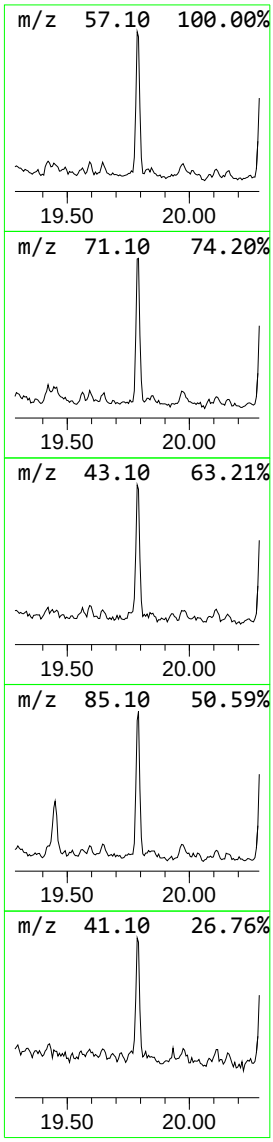
Peak Number 13 Eicosane, 1-iodo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.786	2.09 ng	368935	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86





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Acq On : 20 Aug 2024 22:14
Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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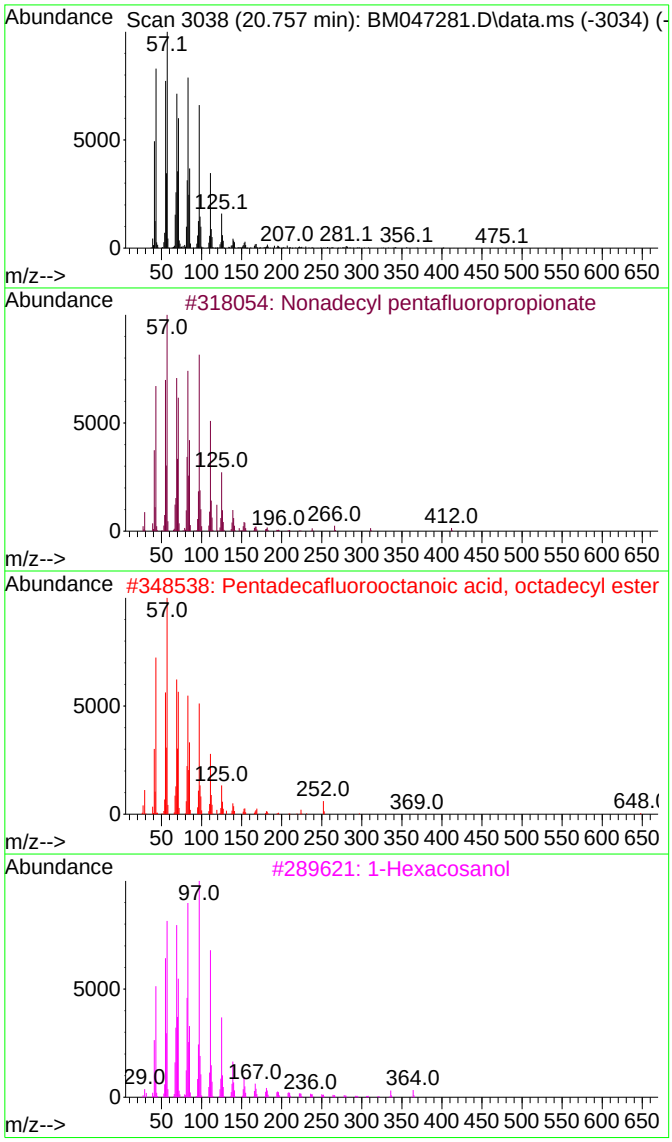
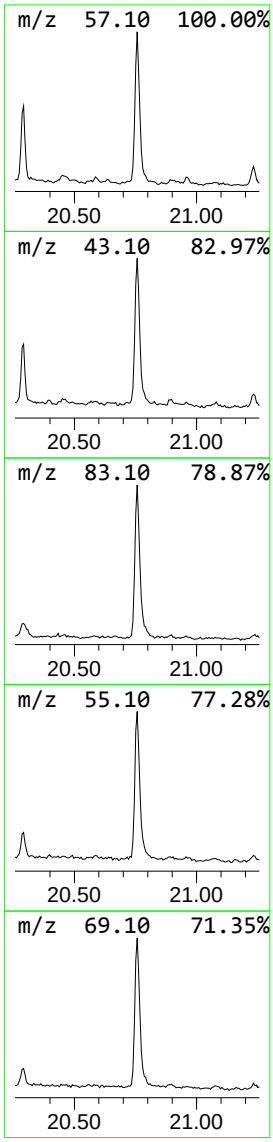
Peak Number 14 Nonadecyl pentafluoropropio... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	6.69 ng	1181200	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91





Tentatively Identified Compound (LSC) summary

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Data File : BM047281.D
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Operator : RC/JU
Sample : P3645-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
916-J-WS-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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	3.264	2.5	ng	216552	1	7.357	1732600	20.0
1-Phenoxypropan...	10.875	2.9	ng	333563	2	10.110	2272510	20.0
Nonadecane	16.574	2.2	ng	392445	4	16.780	3510480	20.0
Heneicosane	17.316	3.6	ng	637755	4	16.780	3510480	20.0
Hexadecanoic ac...	17.492	2.2	ng	385896	4	16.780	3510480	20.0
n-Hexadecanoic ...	17.721	7.1	ng	1243380	4	16.780	3510480	20.0
Eicosane	18.010	4.4	ng	771979	4	16.780	3510480	20.0
Octacosane	18.657	6.8	ng	1194600	4	16.780	3510480	20.0
7-Octadecenoic ...	18.680	2.8	ng	495360	4	16.780	3510480	20.0
Methyl stearate	18.821	2.0	ng	352773	4	16.780	3510480	20.0
Octadecanoic acid	19.015	2.9	ng	514790	5	21.021	3532080	20.0
Tridecane, 1-iodo-	19.245	3.2	ng	566714	5	21.021	3532080	20.0
Eicosane, 1-iodo-	19.786	2.1	ng	368935	5	21.021	3532080	20.0
Nonadecyl penta...	20.756	6.7	ng	1181200	5	21.021	3532080	20.0