LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

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-BM032824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044820.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.505	68	71	81	rBV	55986	88069	1.57%	0.225%
2	5.281	366	373	385	rBV	3161044	4635553	82.73%	11.828%
3	5.687	434	442	447	rBV	31240	56610	1.01%	0.144%
4	6.857	633	641	656	rVB	2957894	4880132	87.10%	12.453%
5	7.328	713	721	728	rBV2	30409	66681	1.19%	0.170%
6	7.669	773	779	786	rVB	527464	801631	14.31%	2.046%
7	8.198	862	869	881	rVB2	31771	64953	1.16%	0.166%
8	8.834	969	977	988	rBV	1846424	3021162	53.92%	7.709%
9	9.481	1083	1087	1096	rVB	33170	57555	1.03%	0.147%
10	10.445	1241	1251	1257	rBV	639035	1087010	19.40%	2.774%
11	12.933	1667	1674	1686	rBV	3839915	5603018	100.00%	14.297%
12	14.033	1857	1861	1869	rVB	40591	65892	1.18%	0.168%
13	14.316	1896	1909	1916	rBV	837640	1436702	25.64%	3.666%
14	15.816	2157	2164	2173	rBV	2750128	3875271	69.16%	9.888%
15	16.980	2358	2362	2369	rBV	48880	72233	1.29%	0.184%
16	17.074	2369	2378	2382	rBV	762593	1202260	21.46%	3.068%
17	17.115	2382	2385	2391	rVB	289013	383431	6.84%	0.978%
18	17.204	2396	2400	2405	rVB	66387	95072	1.70%	0.243%
19	17.862	2506	2512	2517	rVB4	33148	61259	1.09%	0.156%
20	17.921	2517	2522	2524	rBV2	76025	109258	1.95%	0.279%
21	17.980	2528	2532	2543	rVB2	370206	613255	10.95%	1.565%
22	18.145	2554	2560	2564	rBV4	107227	190393	3.40%	0.486%
23	18.180	2564	2566	2573	rVB2	49114	59113	1.06%	0.151%
24	18.268	2576	2581	2587	rBV2	172124	305100	5.45%	0.779%
25	18.415	2602	2606	2609	rBV2	48515	71499	1.28%	0.182%
26	18.698	2651	2654	2659	rVB5	58306	75568	1.35%	0.193%
27	18.821	2671	2675	2680	rVB2	39534	66287	1.18%	0.169%
28	18.874	2680	2684	2690	rBV2	39865	87721	1.57%	0.224%
29	19.104	2719	2723	2725	rBV	159235	191395	3.42%	0.488%
30	19.139	2725	2729	2734	rVB	374894	518099	9.25%	1.322%
31	19.268	2748	2751	2760	rVB2	149110	243532	4.35%	0.621%
32	19.504	2782	2791	2795	rBV	432834	688682	12.29%	1.757%
33	19.715	2821	2827	2832	rVV	3734557	4360846	77.83%	11.127%
34	20.003	2873	2876	2879	rVB2	59805	77537	1.38%	0.198%
35	20.162	2900	2903	2908	rVB	53979	69437	1.24%	0.177%
36	20.268	2917	2921	2924	rBV	208087	263861	4.71%	0.673%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

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-BM032824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.339	2930	2933	2938	rVB3	72631	111098	1.98%	0.283%
38	20.962	3035	3039	3042	rBV2	278117	348678	6.22%	0.890%
39	20.998	3042	3045	3051	rVB3	230109	297050	5.30%	0.758%
40	21.198	3076	3079	3084	rBV	248134	301327	5.38%	0.769%
41	21.268	3085	3091	3095	rVV2	844746	1339651	23.91%	3.418%
42	21.303	3095	3097	3105	rVB	214720	295263	5.27%	0.753%
43	23.503	3466	3471	3478	rVB	520996	950694	16.97%	2.426%

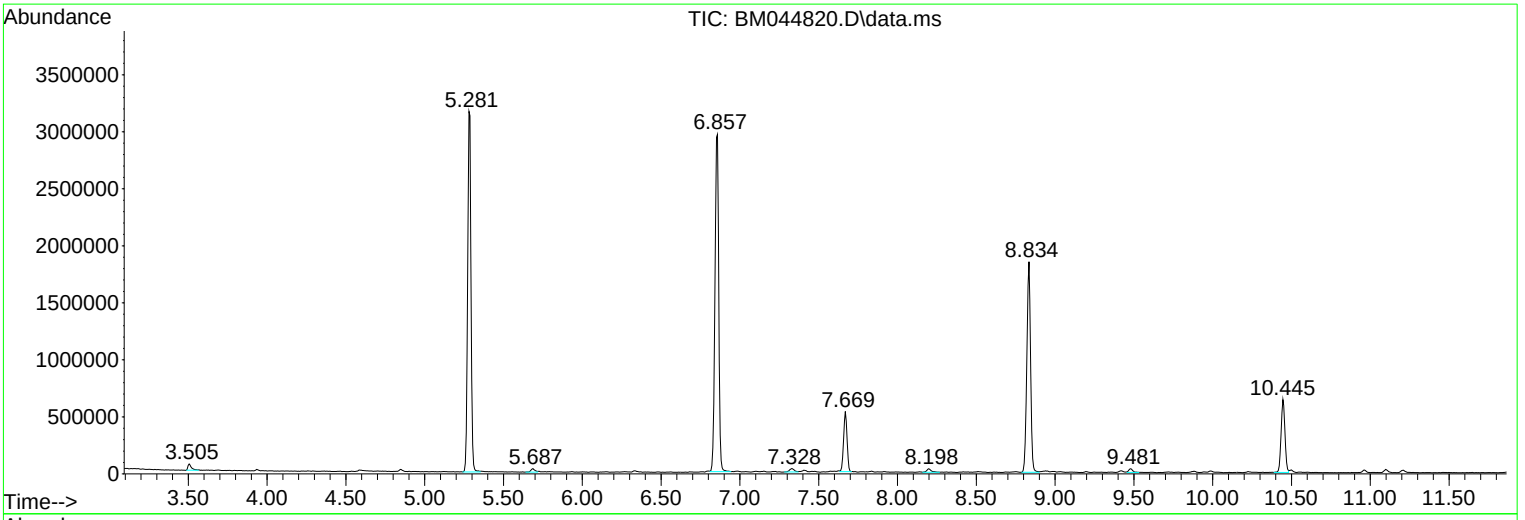
Sum of corrected areas: 39189838

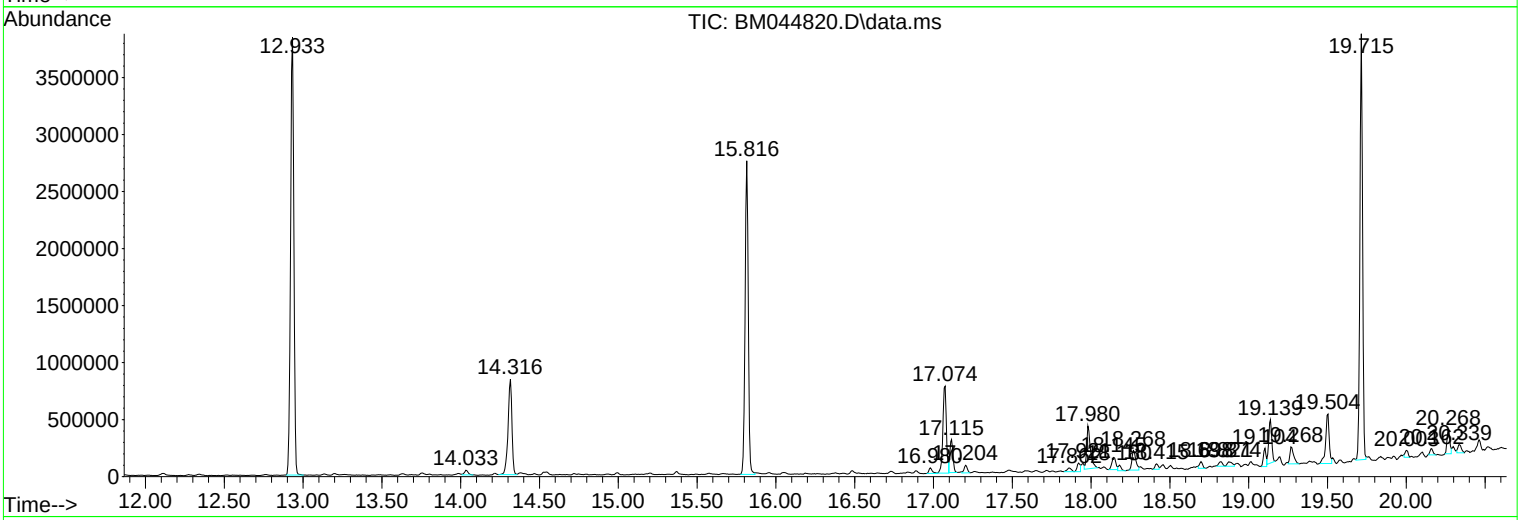
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

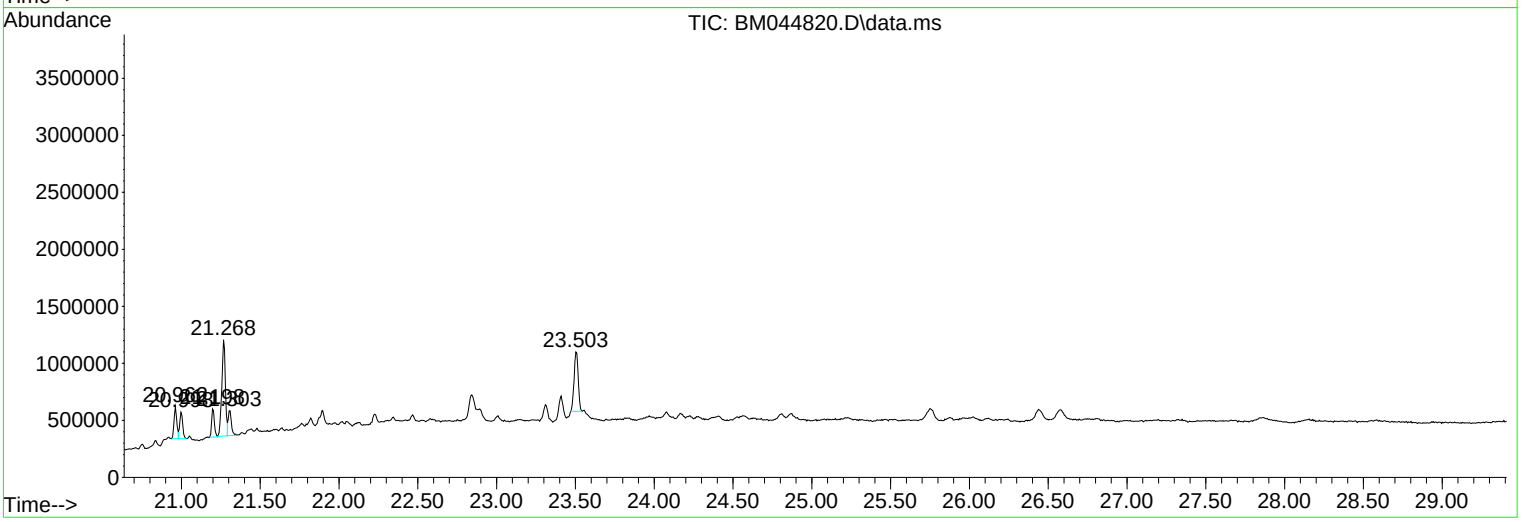
Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

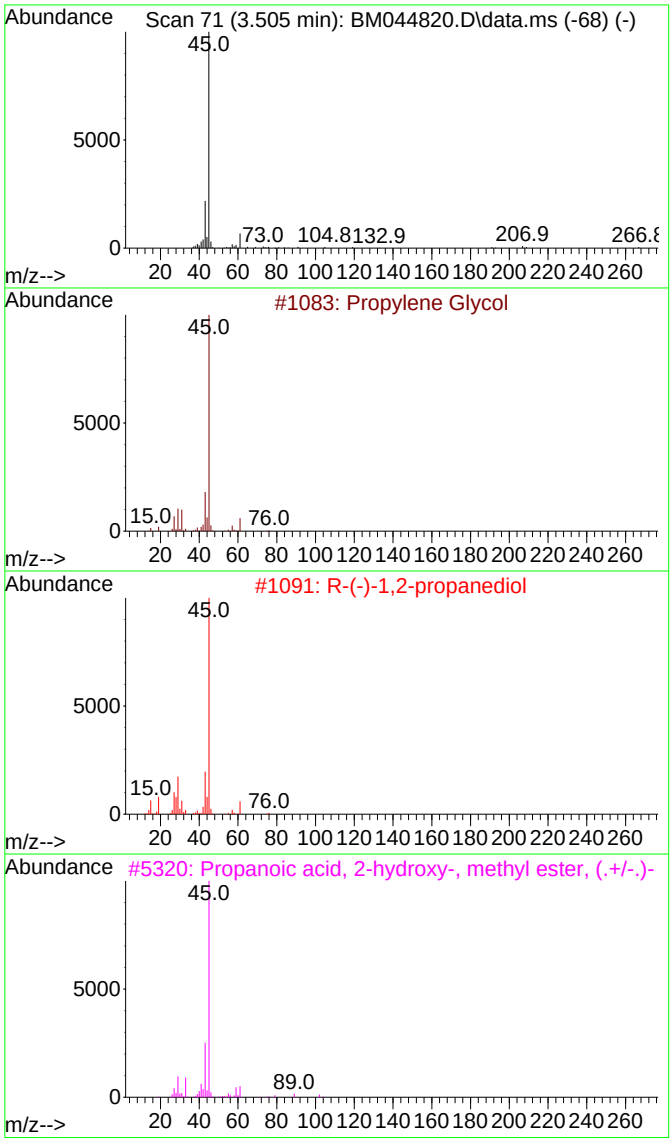
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

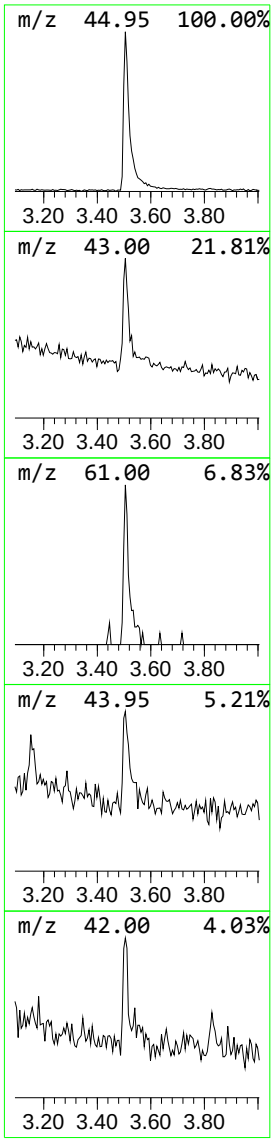
****

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.505	2.20 ng	88069	1,4-Dichlorobenzene-d4	7.669

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	72
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

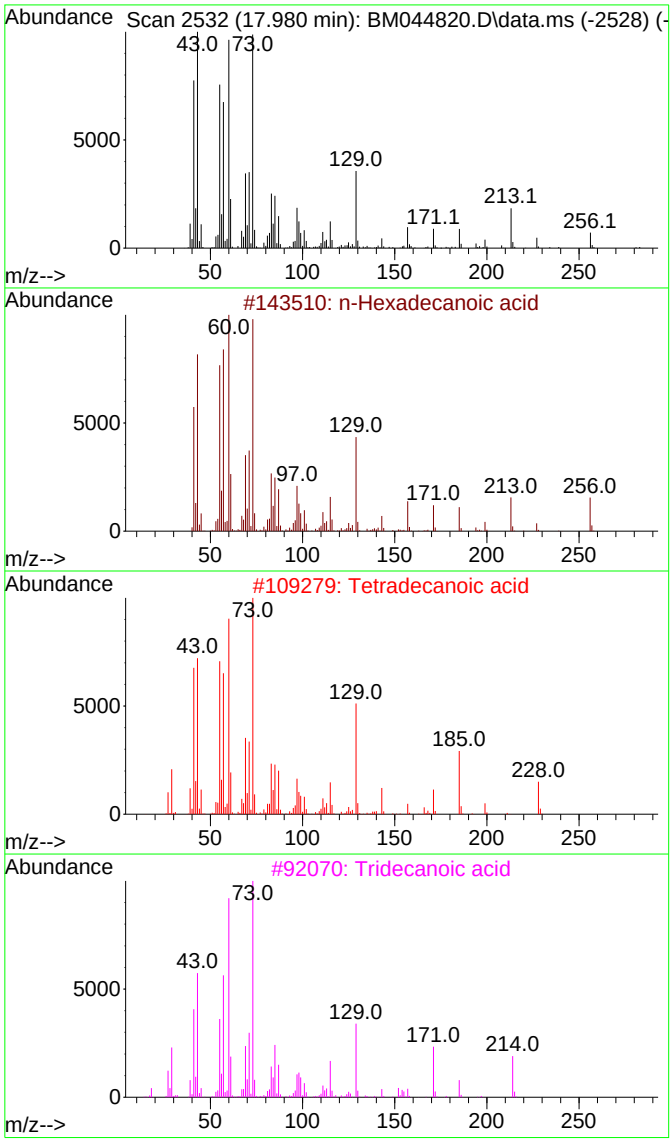
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

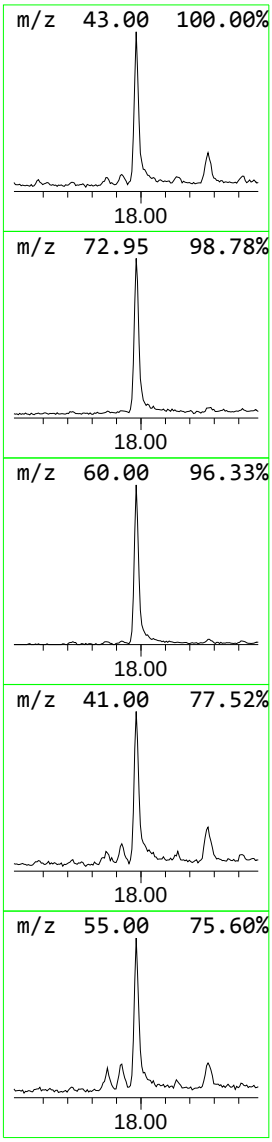
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	10.20 ng	613255	Phenanthrene-d10	17.074

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

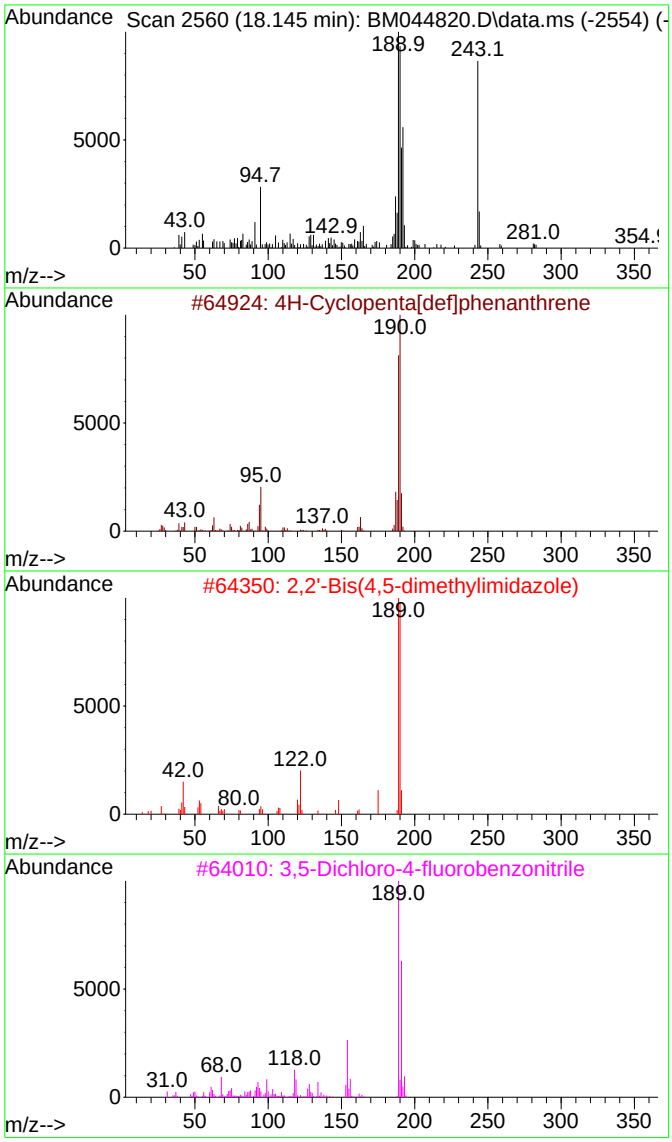
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

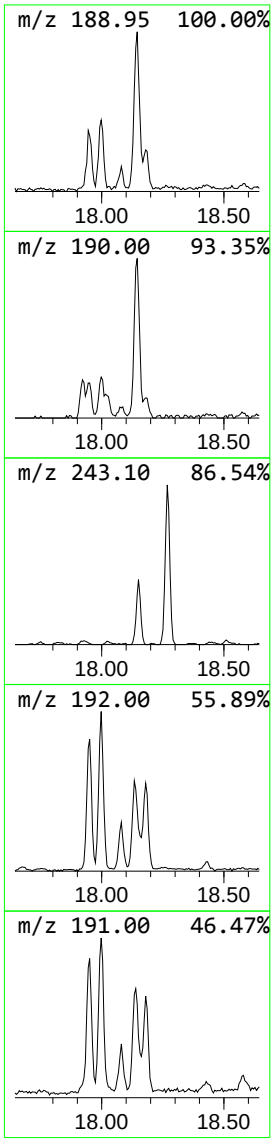
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	3.17 ng	190393	Phenanthrene-d10	17.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	35
3	3,5-Dichloro-4-fluorobenzonitrile	189	C7H2Cl2FN	103879-31-8	25
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	25
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

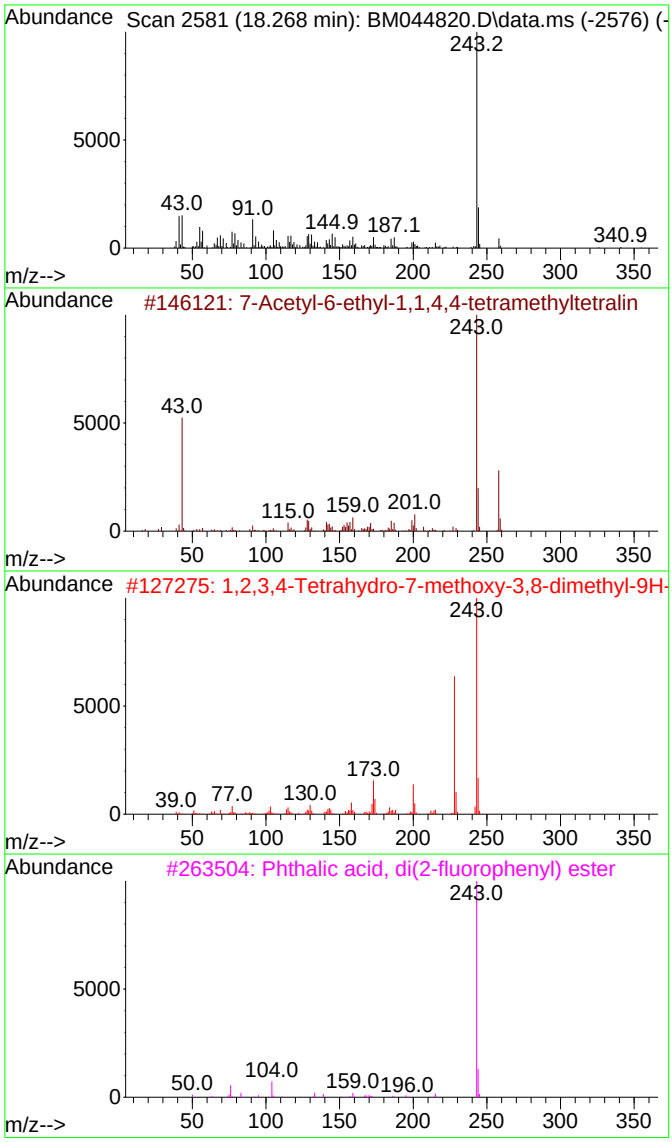
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

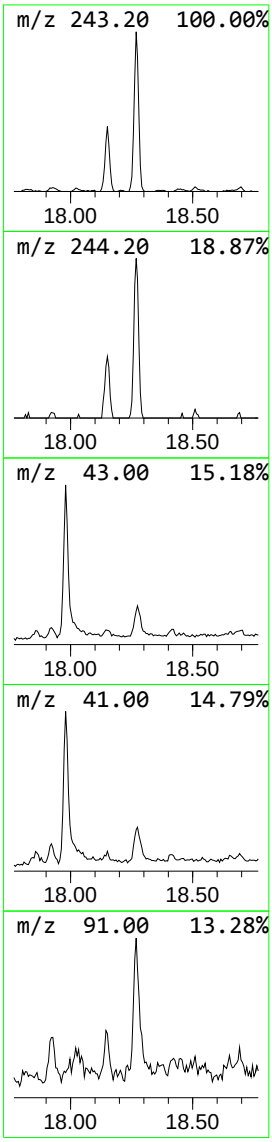
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7-Acetyl-6-ethyl-1,1,4,4-te... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	5.08 ng	305100	Phenanthrene-d10	17.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Acetyl-6-ethyl-1,1,4,4-tetrame...	258	C18H26O	000088-29-9	72
2	1,2,3,4-Tetrahydro-7-methoxy-3,8...	243	C15H17NO2	1000281-20-4	64
3	Phthalic acid, di(2-fluorophenyl...	354	C20H12F2O4	1000356-50-0	64
4	3-Phenyl-4-azafluorene	243	C18H13N	033777-97-8	59
5	2-Aminochrysene	243	C18H13N	000789-47-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

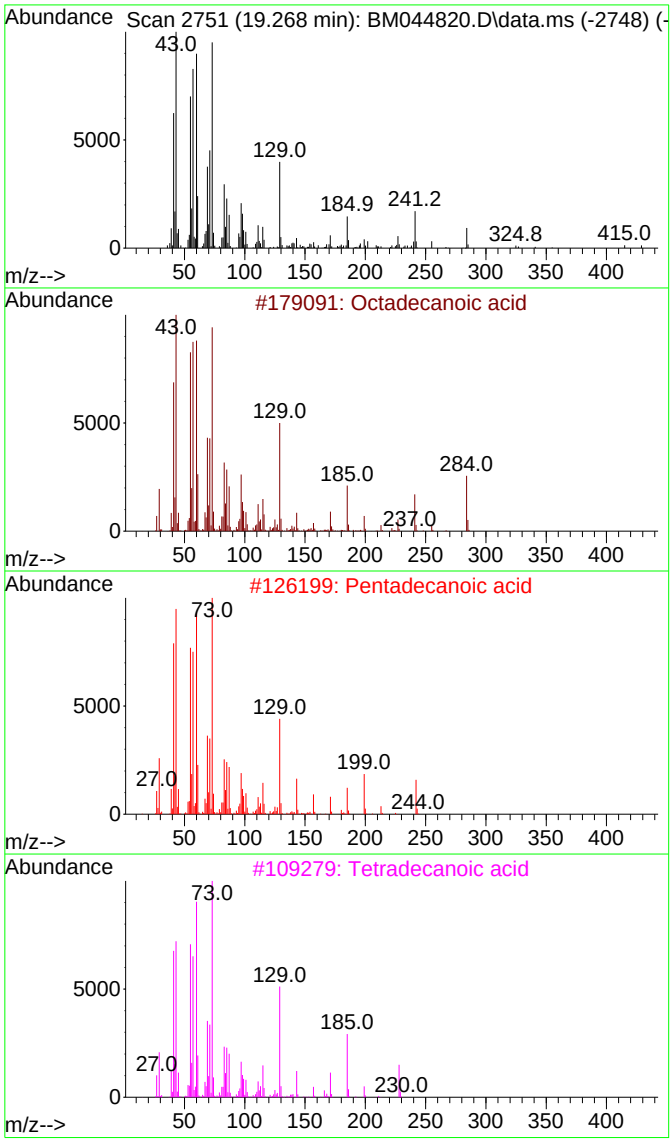
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

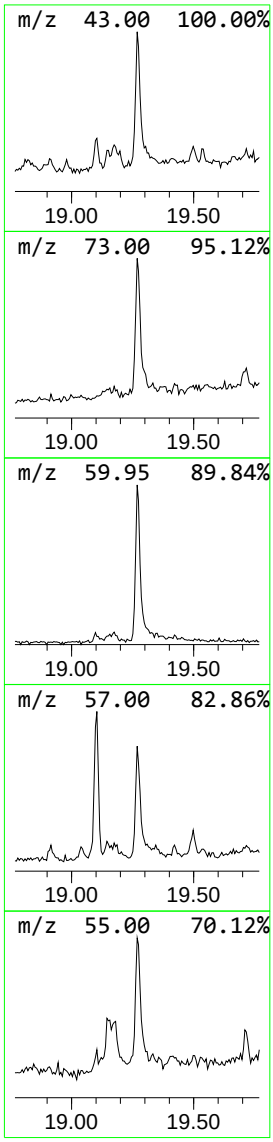
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	3.64 ng	243532	Chrysene-d12	21.268

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Octanoic acid	144	C8H16O2	000124-07-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

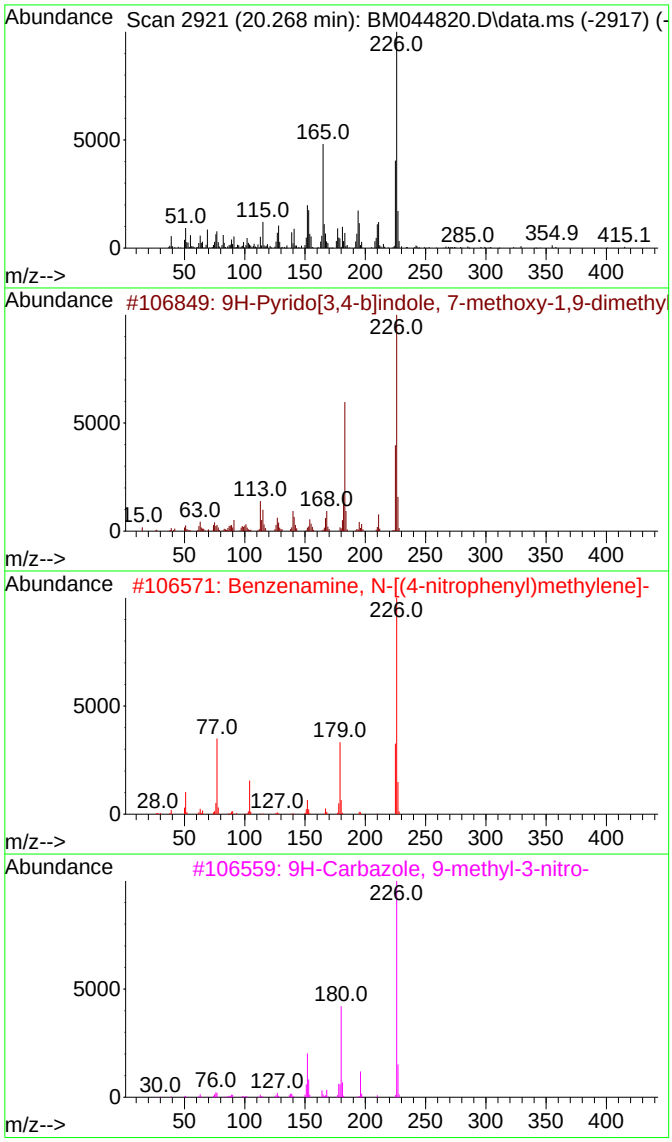
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

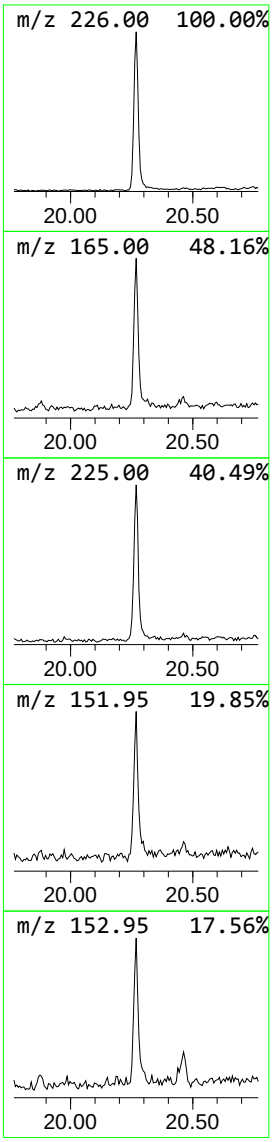
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9H-Pyrido[3,4-b]indole, 7-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.268	3.94 ng	263861	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	58
2	Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	46
3	9H-Carbazole, 9-methyl-3-nitro-	226	C13H10N2O2	061166-05-0	45
4	1-Ethyl-4-methoxy-9H-pyrido[3,4-...	226	C14H14N2O	026585-14-8	43
5	Anthralin	226	C14H10O3	001143-38-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
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Misc :
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Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

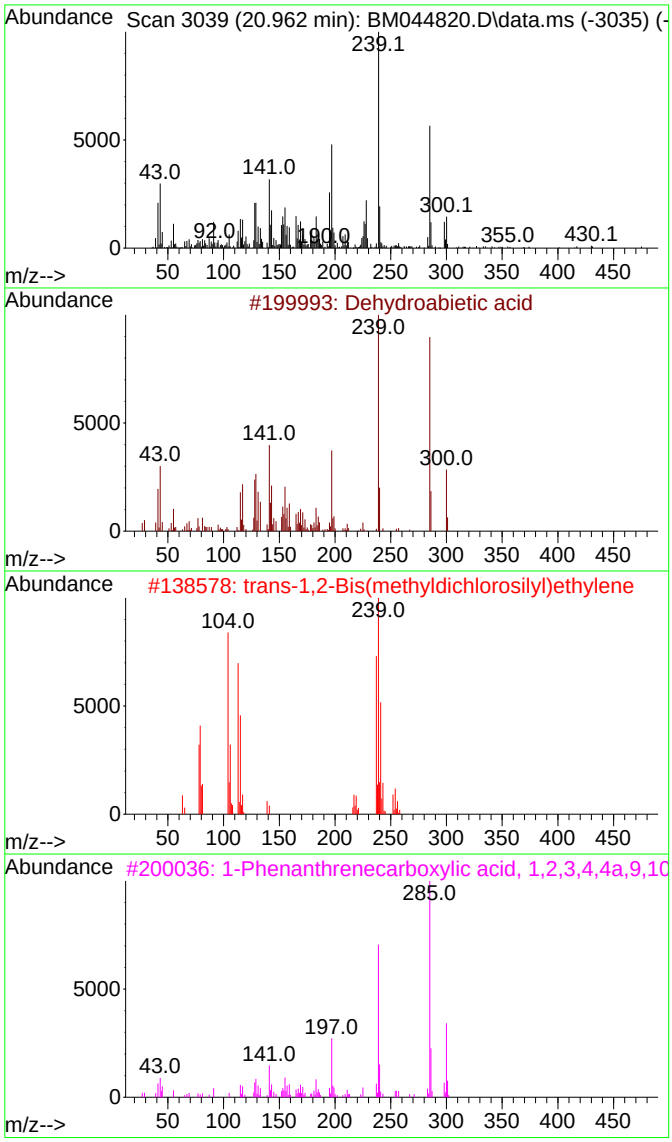
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

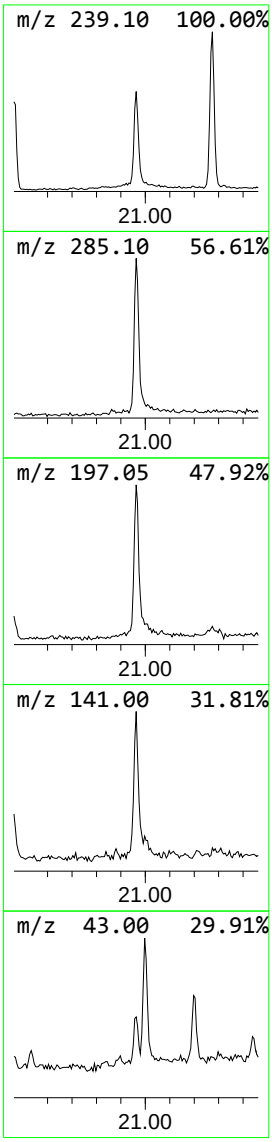
****

Peak Number 7 Dehydroabietic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.962	5.21 ng	348678	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydroabietic acid	300	C20H28O2	001740-19-8	99
2	trans-1,2-Bis(methyldichlorosily...	252	C4H8Cl4Si2	065899-10-7	92
3	1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	90
4	2-Phenyl-4-(propen-1-yl)-pyrimid...	239	C14H13N3O	1010287-21-7	86
5	Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

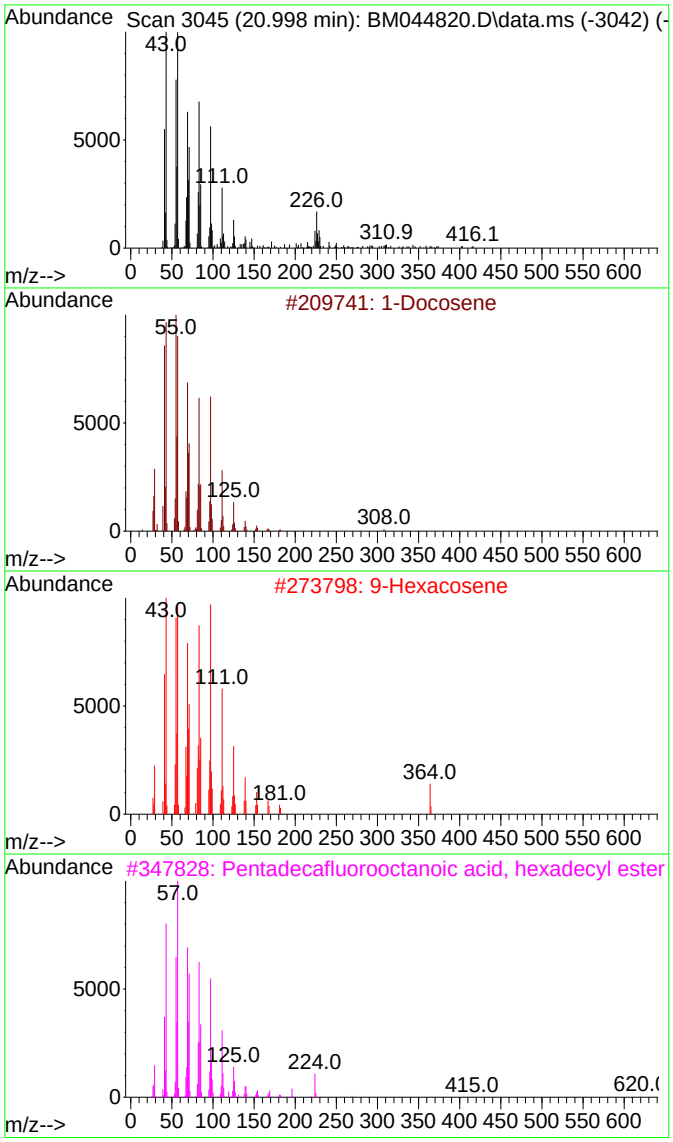
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

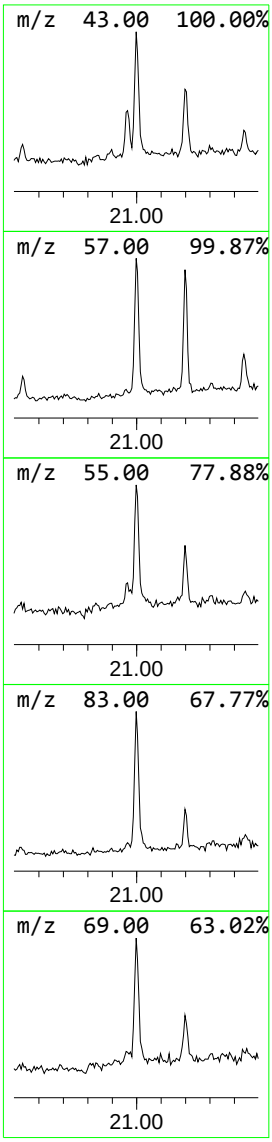
****

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.997	4.43 ng	297050	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	9-Hexacosene	364	C26H52	071502-22-2	93
3	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	93
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	Cyclotetracosane	336	C24H48	000297-03-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044820.D
Acq On : 29 Mar 2024 18:14
Operator : MA/JU
Sample : P1879-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-04(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.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	3.505	2.2	ng	88069	1	7.669	801631	20.0
n-Hexadecanoic ...	17.980	10.2	ng	613255	4	17.074	1202260	20.0
4H-Cyclopenta[d...	18.145	3.2	ng	190393	4	17.074	1202260	20.0
7-Acetyl-6-ethy...	18.268	5.1	ng	305100	4	17.074	1202260	20.0
Octadecanoic acid	19.268	3.6	ng	243532	5	21.268	1339650	20.0
9H-Pyrido[3,4-b...	20.268	3.9	ng	263861	5	21.268	1339650	20.0
Dehydroabietic ...	20.962	5.2	ng	348678	5	21.268	1339650	20.0
1-Docosene	20.997	4.4	ng	297050	5	21.268	1339650	20.0