LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.952	294	300	309	rBV	1375087	1929575	25.18%	2.922%
2	5.422	374	380	399	rBV	2906595	4586366	59.84%	6.946%
3	7.040	643	655	678	rBV	2827054	4861713	63.43%	7.363%
4	7.863	787	795	810	rBV	800474	1369111	17.86%	2.074%
5	9.034	987	994	1013	rBV	1688177	3007823	39.24%	4.555%
6	10.675	1261	1273	1279	rBV	1063317	1931126	25.20%	2.925%
7	11.863	1466	1475	1483	rBV3	50157	115911	1.51%	0.176%
8	12.092	1506	1514	1518	rBV3	43055	78459	1.02%	0.119%
9	13.139	1685	1692	1702	rBV	4375988	6399778	83.50%	9.692%
10	13.333	1721	1725	1732	rVB2	79716	128358	1.67%	0.194%
11	13.992	1831	1837	1840	rBV2	59167	98557	1.29%	0.149%
12	14.239	1875	1879	1886	rBV	85469	146973	1.92%	0.223%
13	14.410	1903	1908	1913	rVB	203761	258465	3.37%	0.391%
14	14.516	1917	1926	1933	rVV	1646079	2552949	33.31%	3.866%
15	14.580	1934	1937	1944	rVB2	75028	125431	1.64%	0.190%
16	14.916	1990	1994	2000	rBV3	64117	103894	1.36%	0.157%
17	15.027	2010	2013	2018	rVB3	56310	84541	1.10%	0.128%
18	15.363	2065	2070	2075	rVB	344284	427161	5.57%	0.647%
19	15.769	2135	2139	2144	rVB	133319	195737	2.55%	0.296%
20	15.880	2152	2158	2162	rBV	197178	299650	3.91%	0.454%
21	16.010	2172	2180	2188	rBV	3382976	5062091	66.05%	7.667%
22	16.221	2212	2216	2233	rBV	500828	1047788	13.67%	1.587%
23	17.021	2347	2352	2356	rBV	505406	651077	8.49%	0.986%
24	17.068	2357	2360	2371	rVB2	231947	465514	6.07%	0.705%
25	17.268	2389	2394	2398	rBV	1914561	2759888	36.01%	4.180%
26	17.310	2398	2401	2409	rVV	953990	1395136	18.20%	2.113%
27	17.398	2413	2416	2421	rVB	193292	279832	3.65%	0.424%
28	17.680	2461	2464	2471	rVB	115195	175917	2.30%	0.266%
29	17.763	2474	2478	2488	rVB	473637	633606	8.27%	0.960%
30	18.168	2543	2547	2558	rVB2	1220078	2053289	26.79%	3.110%
31	18.457	2592	2596	2601	rBV	493173	658365	8.59%	0.997%
32	19.092	2701	2704	2708	rVB	330021	352966	4.61%	0.535%
33	19.333	2740	2745	2751	rVB	2138103	2972938	38.79%	4.502%
34	19.451	2761	2765	2769	rBV	631125	954691	12.46%	1.446%
35	19.668	2799	2802	2803	rBV2	434464	469145	6.12%	0.711%
36	19.692	2803	2806	2815	rVB	1632508	2331258	30.42%	3.531%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.898	2836	2841	2852	rBV	6013779	7664455	100.00%	11.608%
38	21.462	3101	3107	3111	rBV2	2726992	4808358	62.74%	7.282%
39	23.856	3509	3514	3520	rVB2	1405616	2590812	33.80%	3.924%

Sum of corrected areas: 66028704

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
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Misc :
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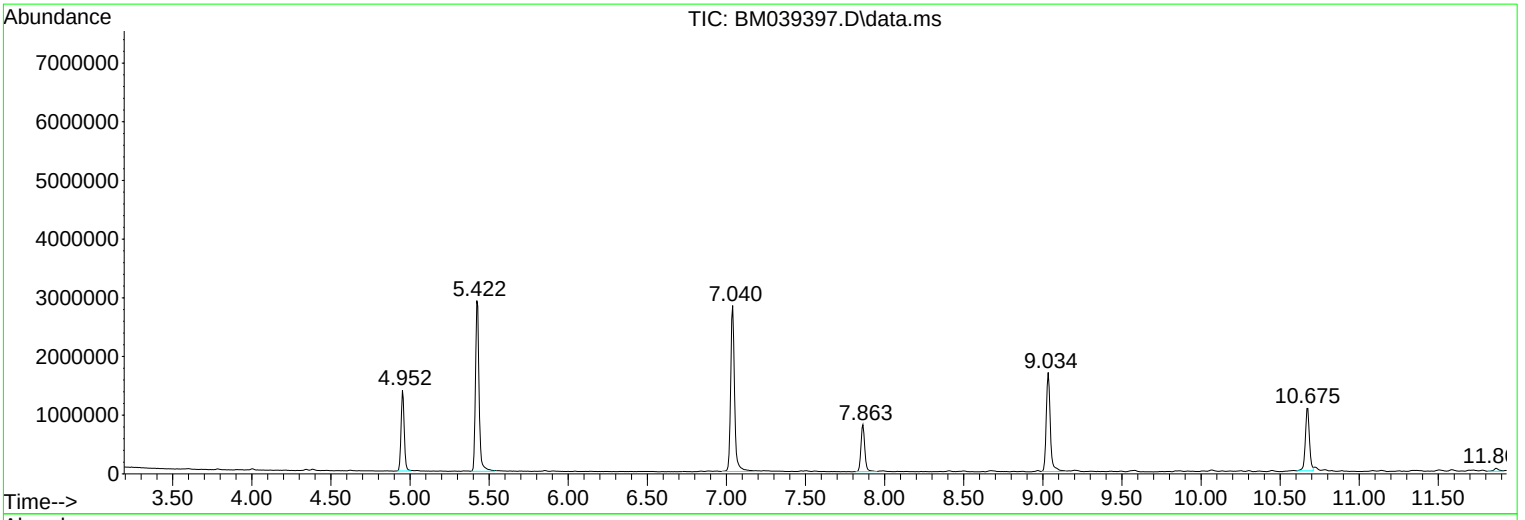
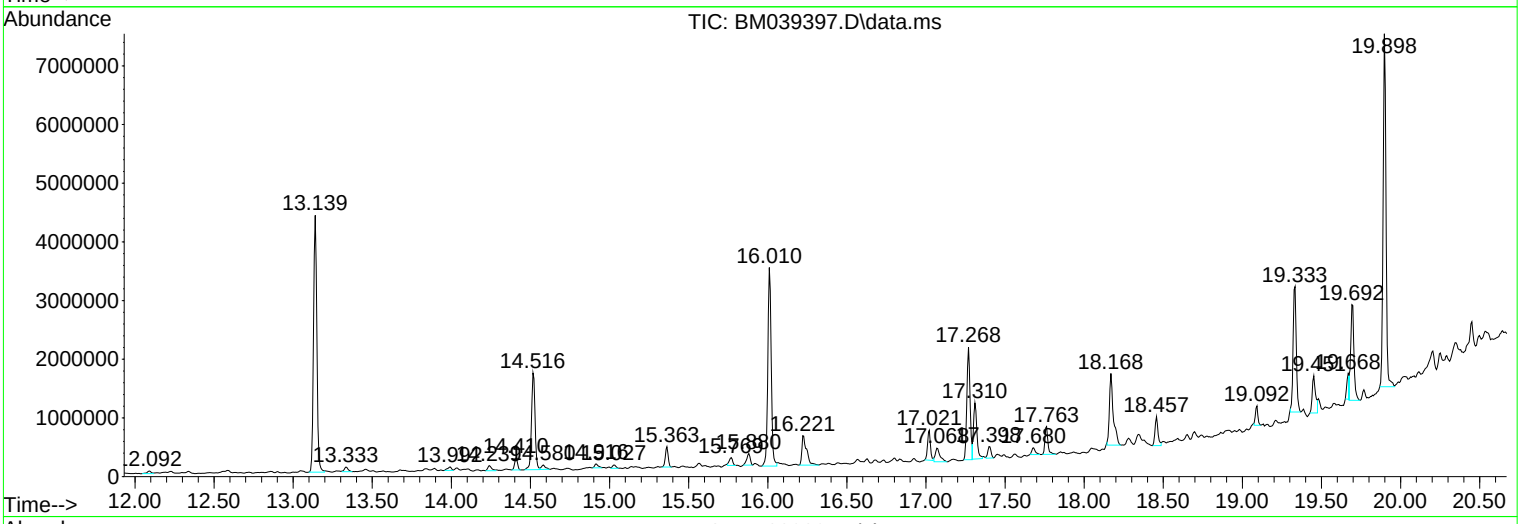
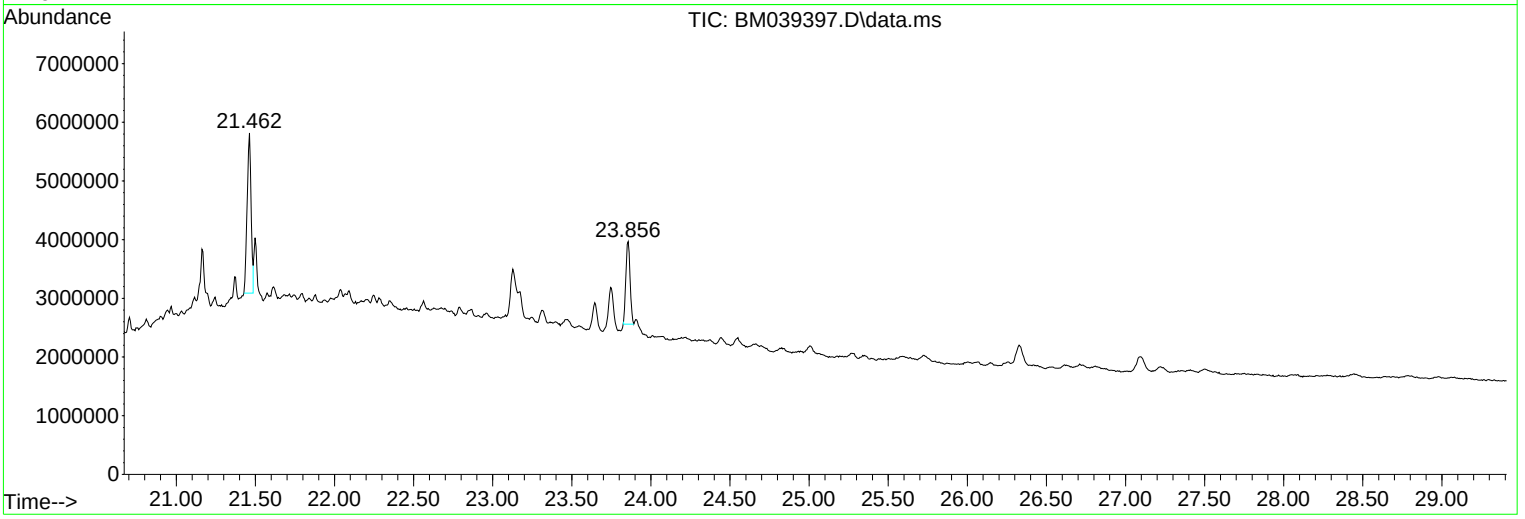
Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

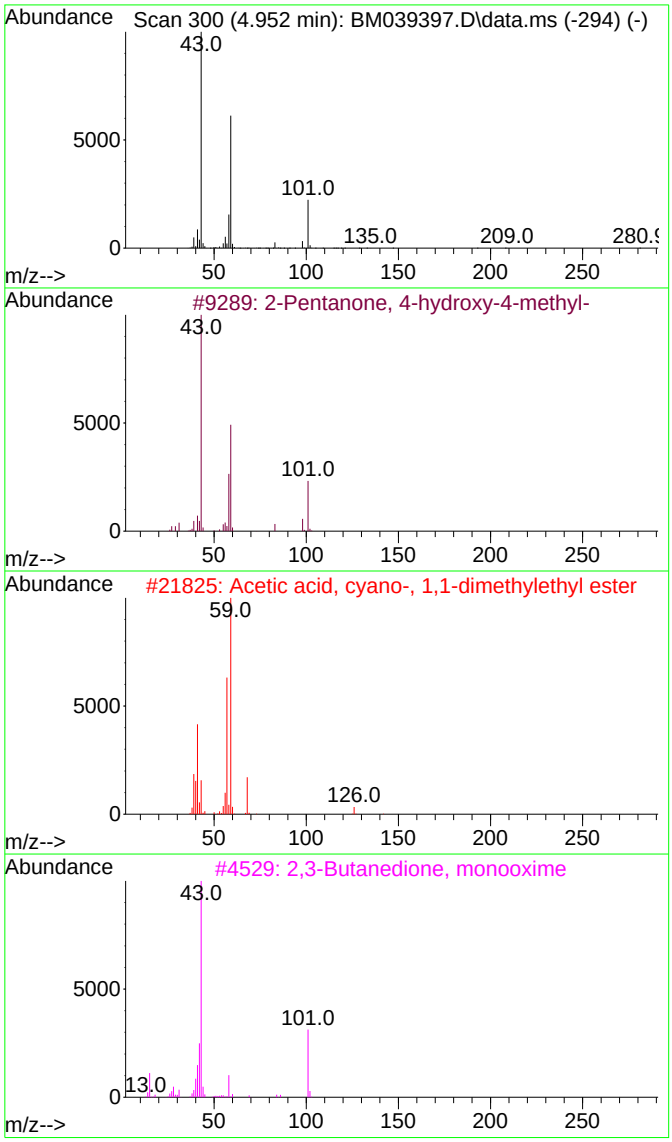
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

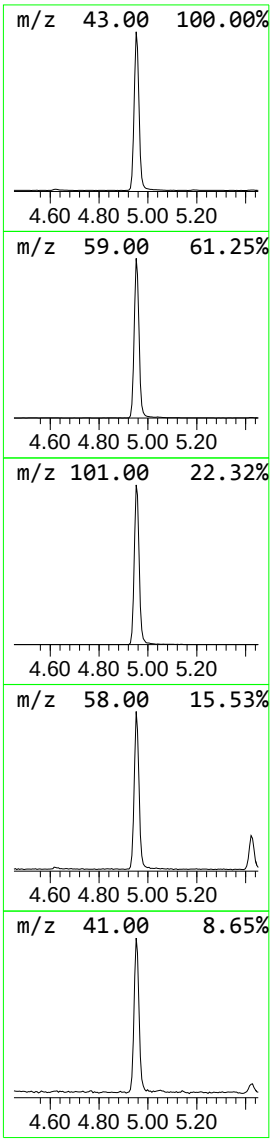
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	28.19 ng	1929580	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

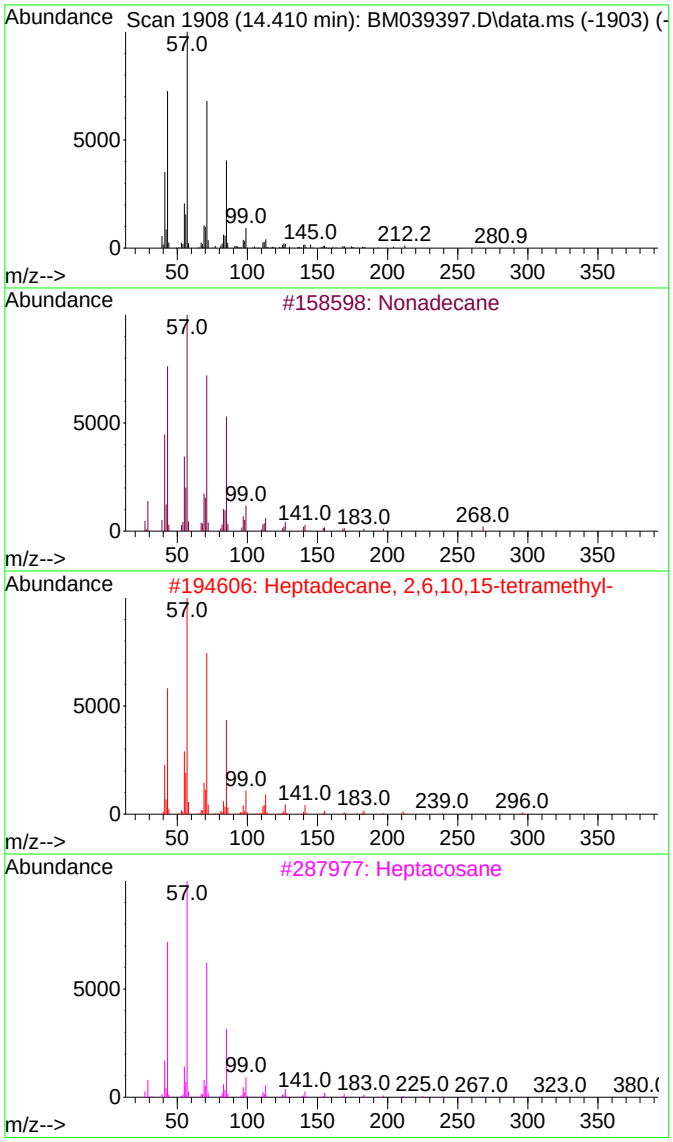
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

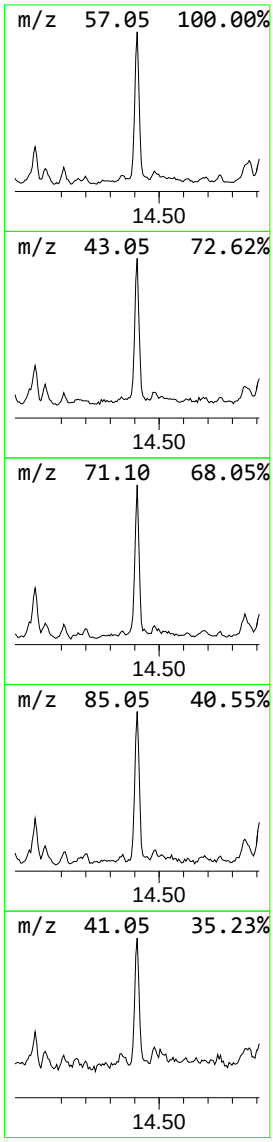
****

Peak Number 2 Nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	2.02 ng	258465	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

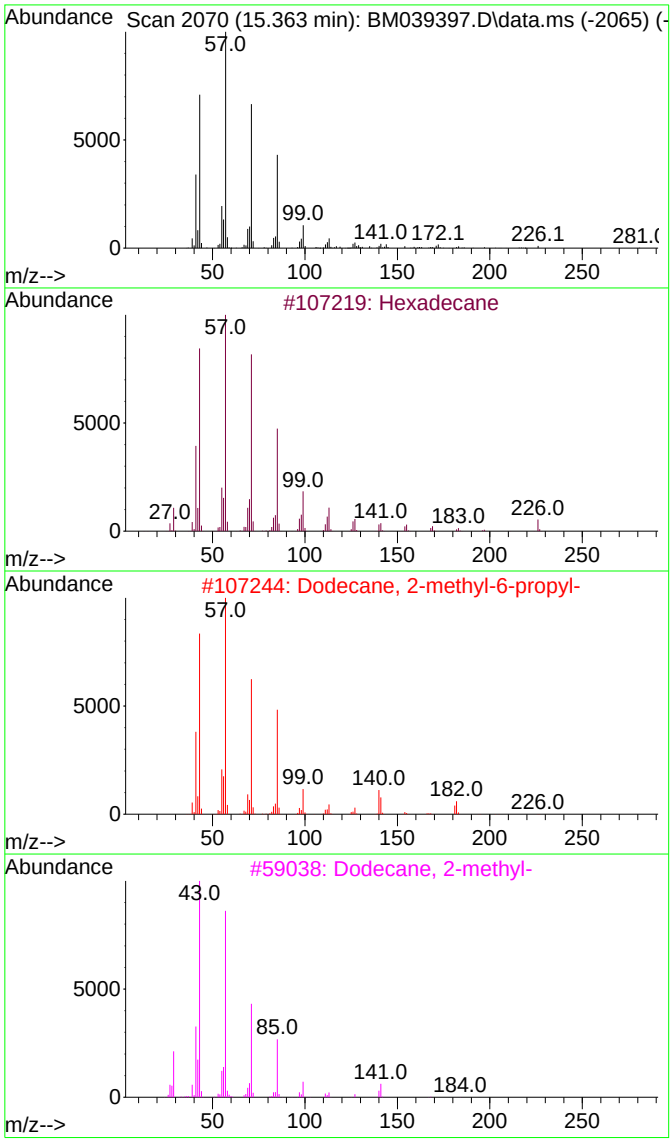
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

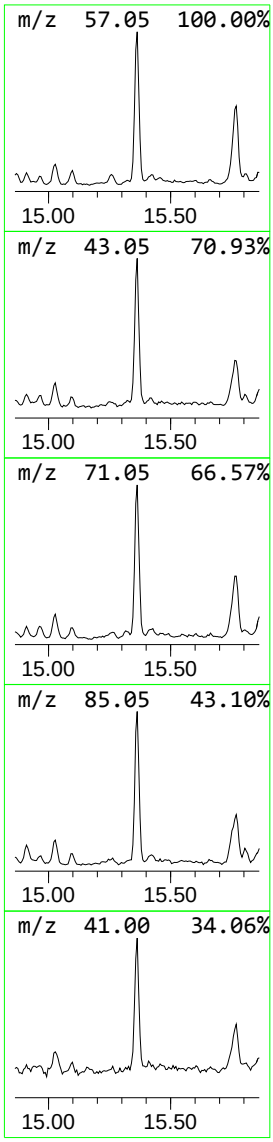
****

Peak Number 3 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	3.35 ng	427161	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Tridecane	184	C13H28	000629-50-5	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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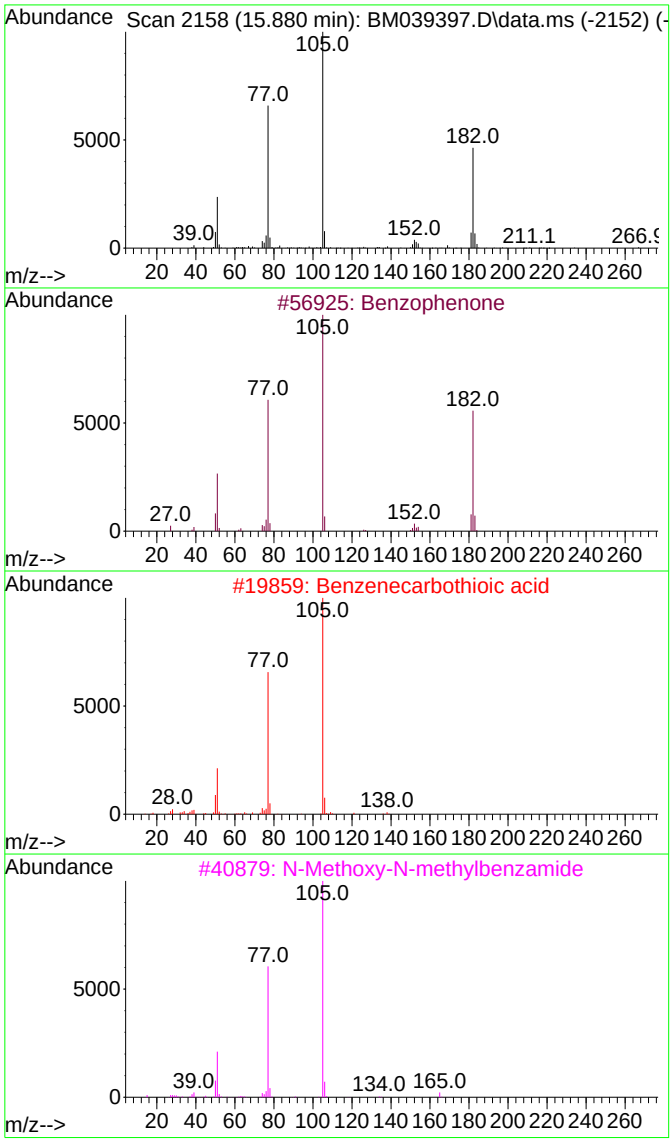
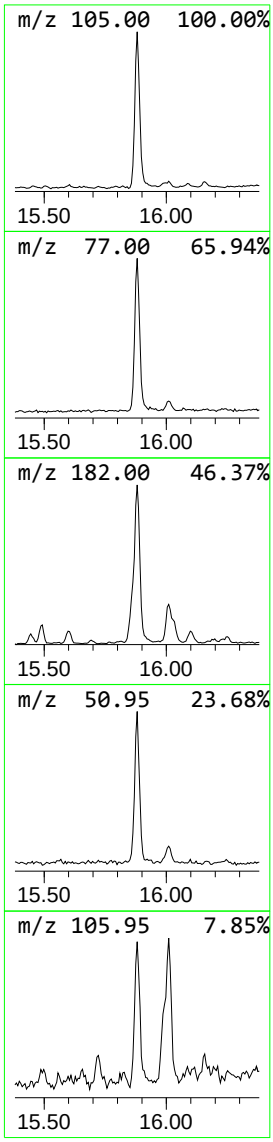
Peak Number 4 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	2.35 ng	299650	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	49
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
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Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

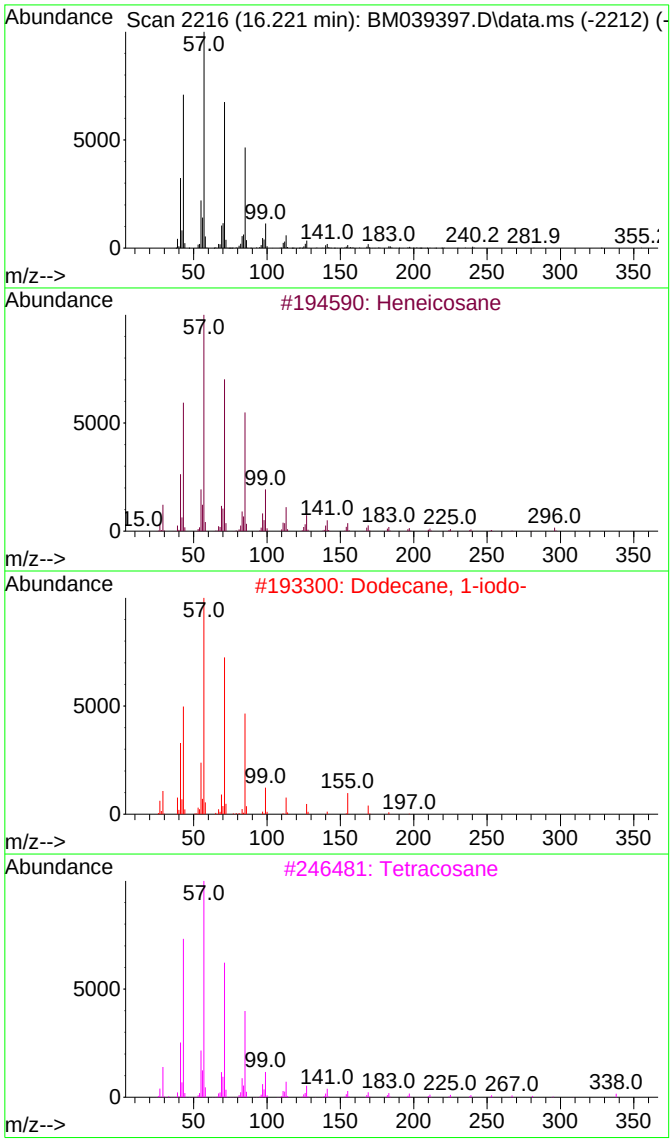
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

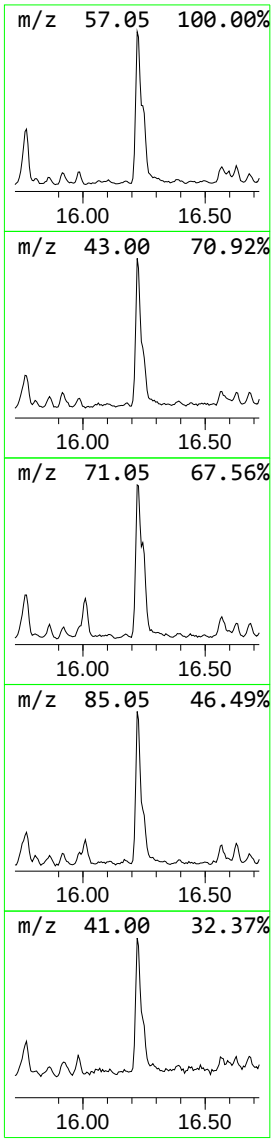
****

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	7.59 ng	1047790	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Tetradecane	198	C14H30	000629-59-4	86





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Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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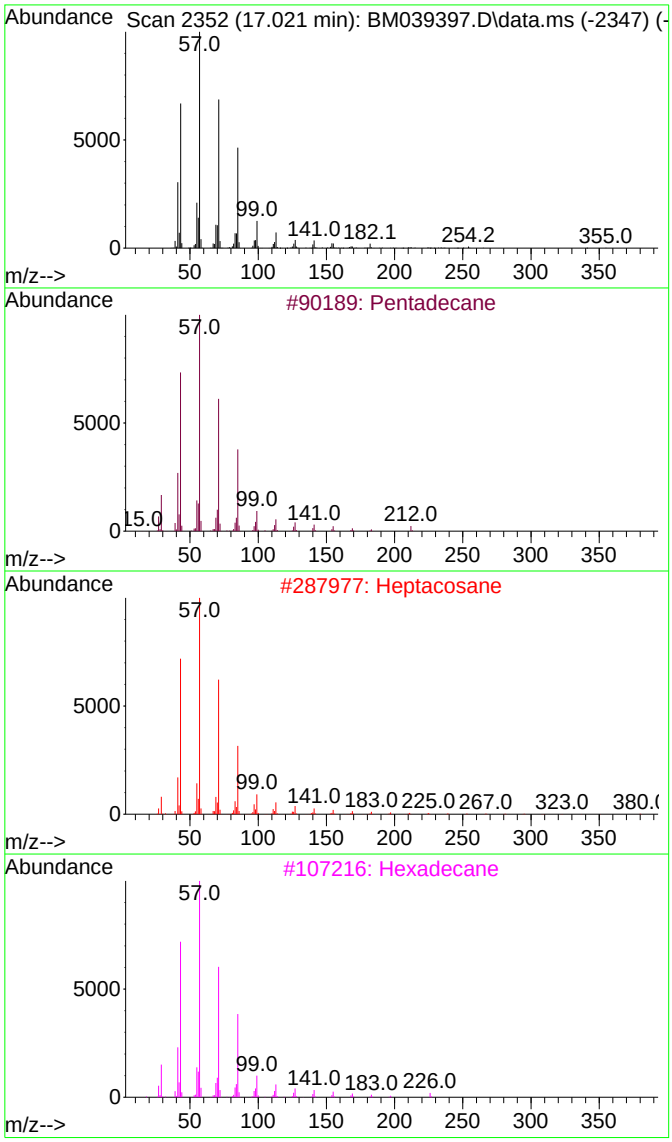
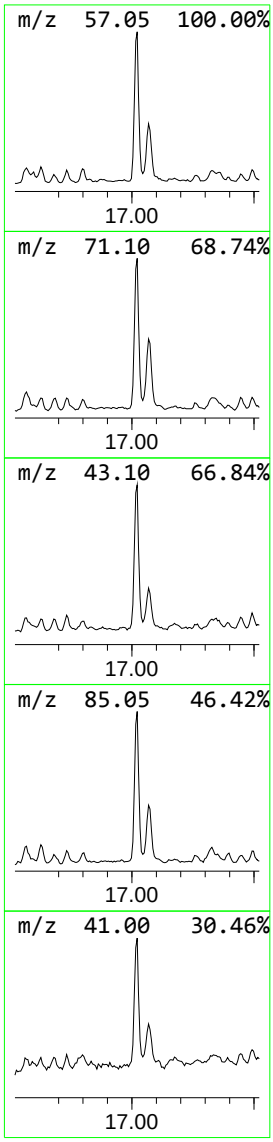
Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.021	4.72 ng	651077	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Nonadecane	268	C19H40	000629-92-5	90





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

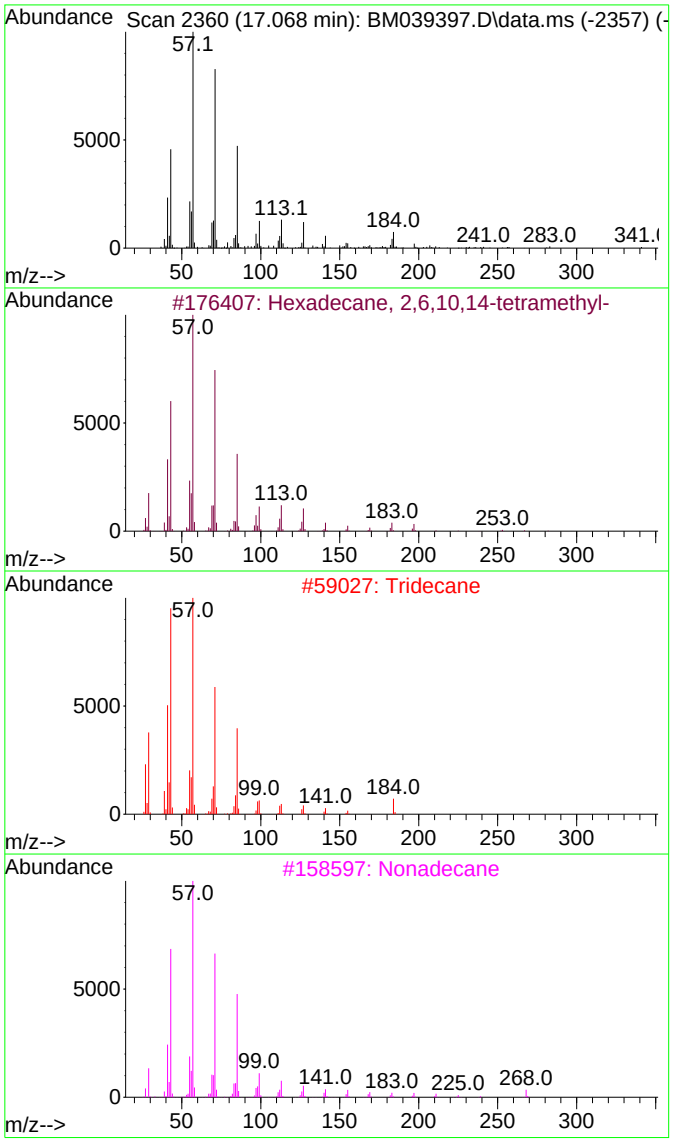
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

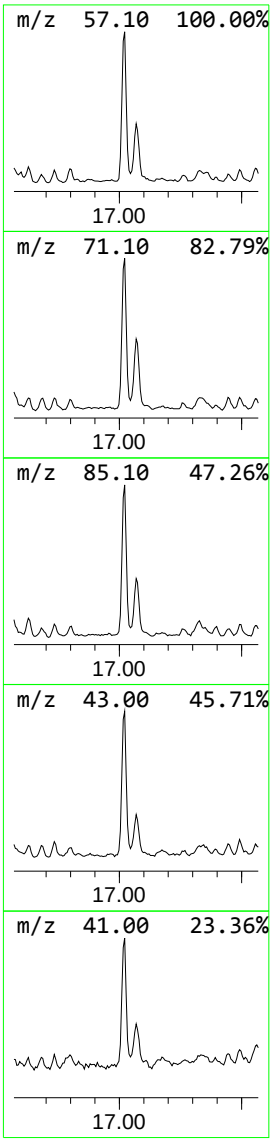
****

Peak Number 7 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.069	3.37 ng	465514	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

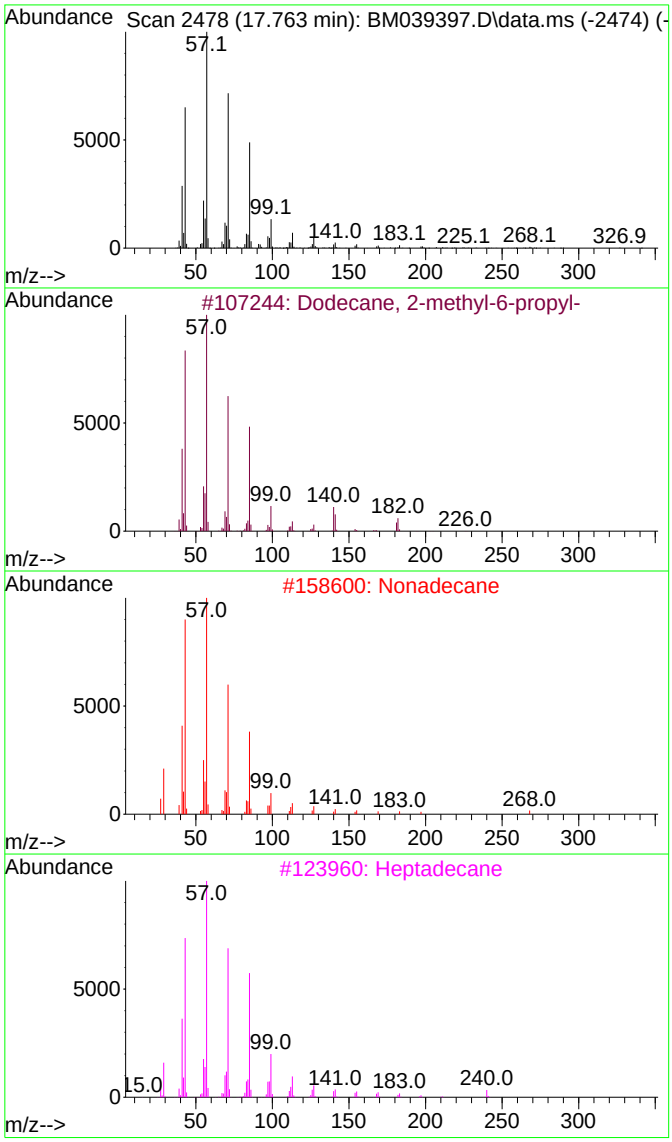
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

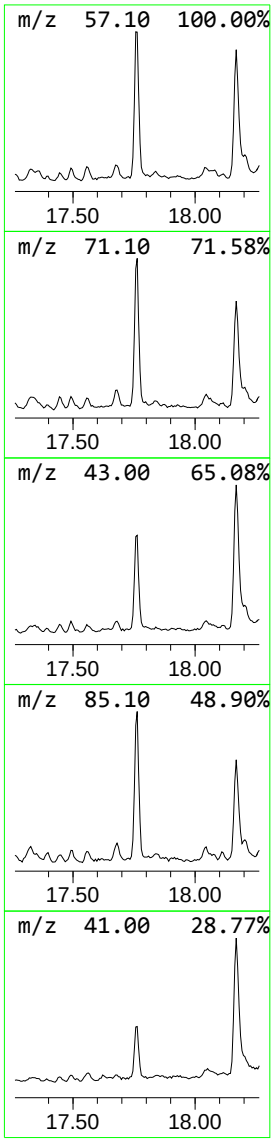
****

Peak Number 8 Dodecane, 2-methyl-6-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.763	4.59 ng	633606	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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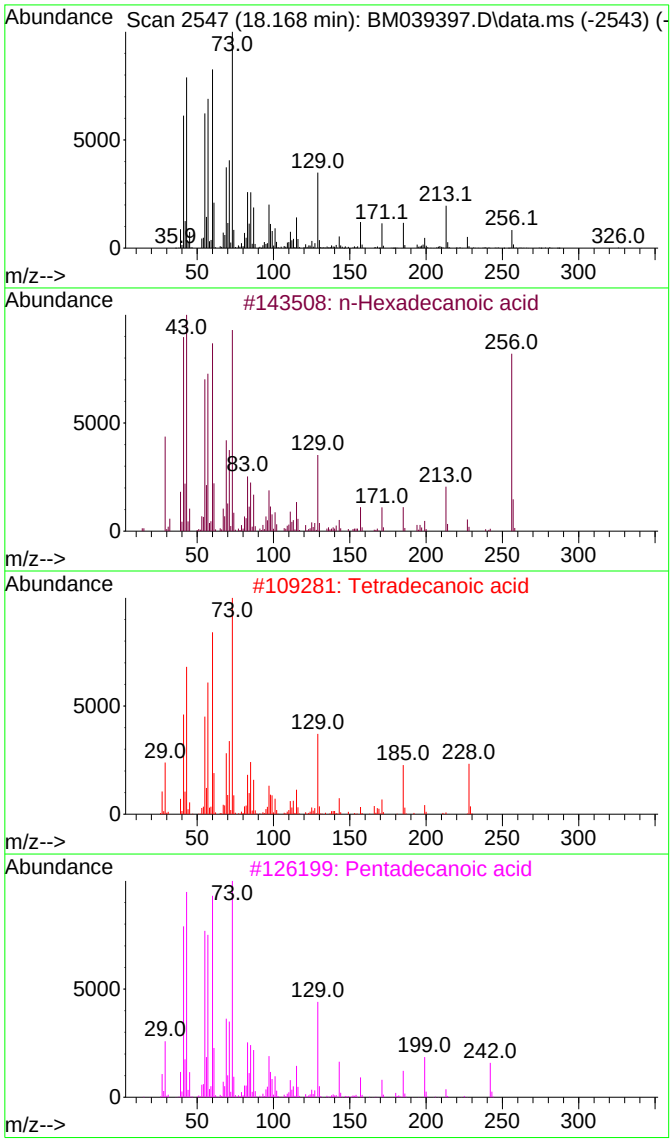
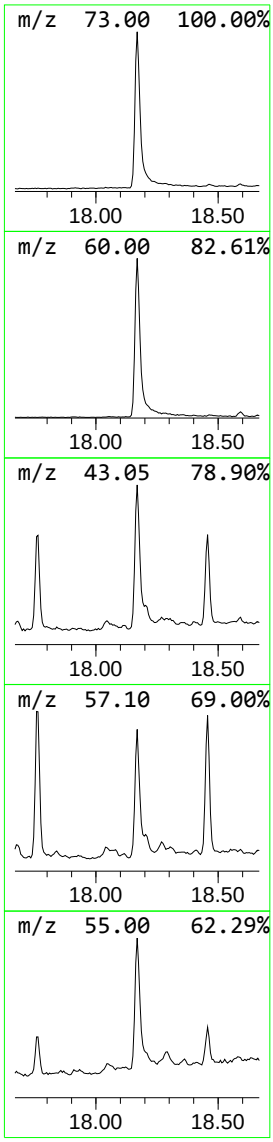
Peak Number 9 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	14.88 ng	2053290	Phenanthrene-d10	17.269

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





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Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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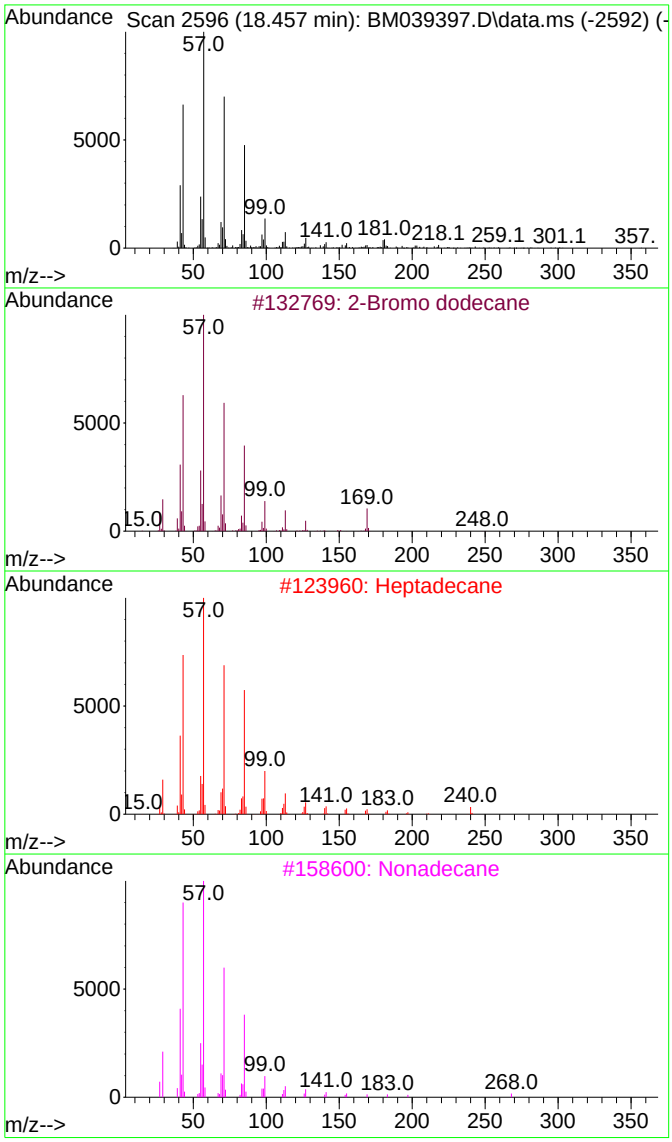
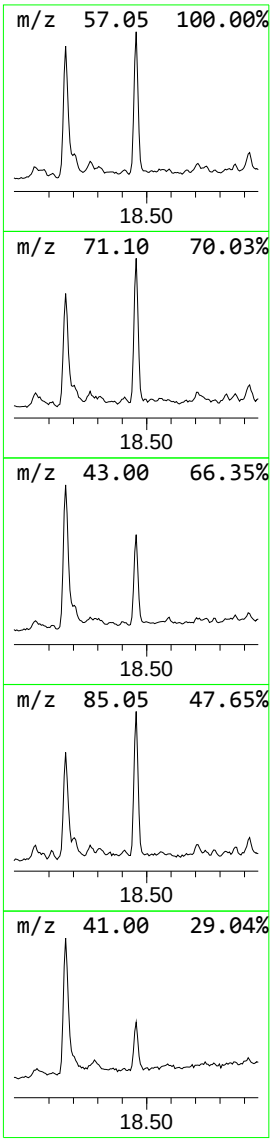
Peak Number 10 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.457	4.77 ng	658365	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
2	Heptadecane	240	C17H36	000629-78-7	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Pentacosane	352	C25H52	000629-99-2	87





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Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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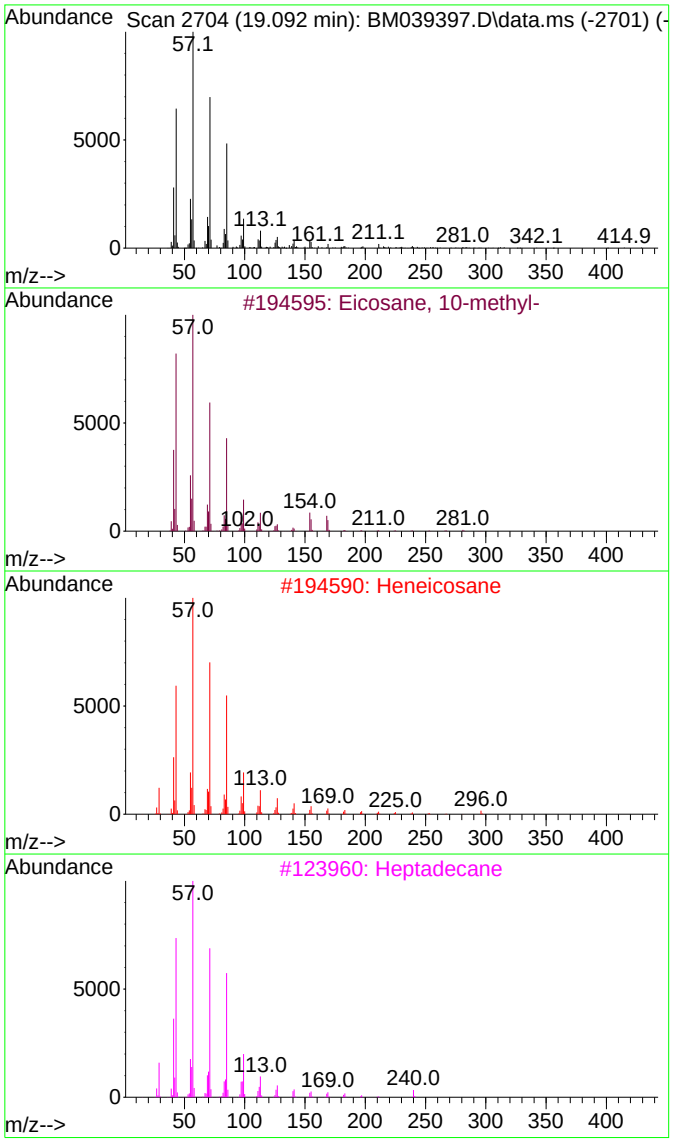
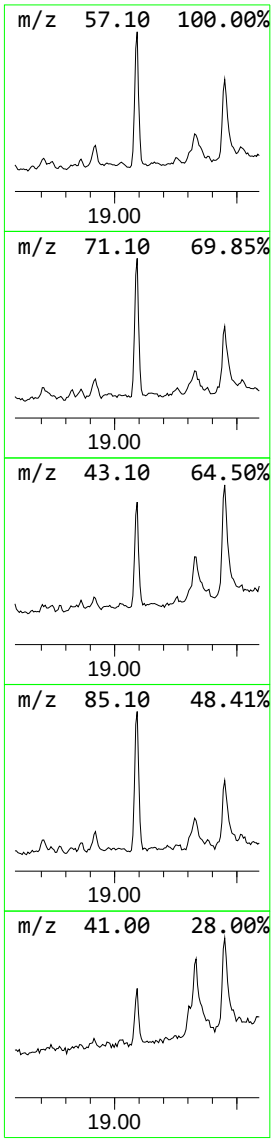
Peak Number 11 Eicosane, 10-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.092	2.56 ng	352966	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5	Hexadecane	226	C16H34	000544-76-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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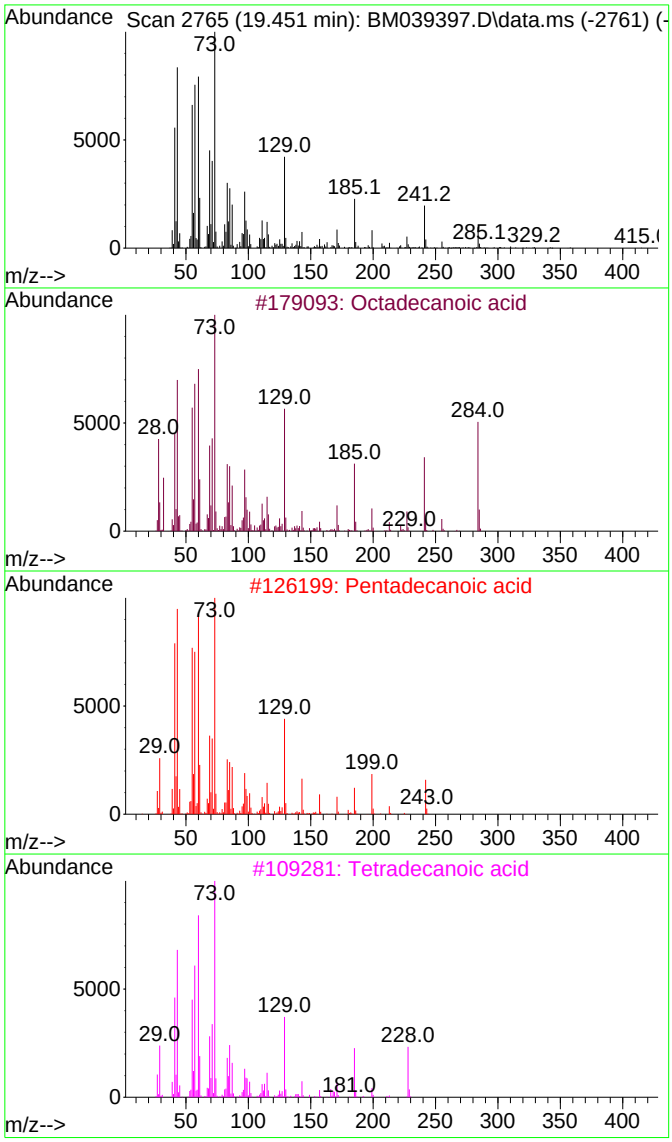
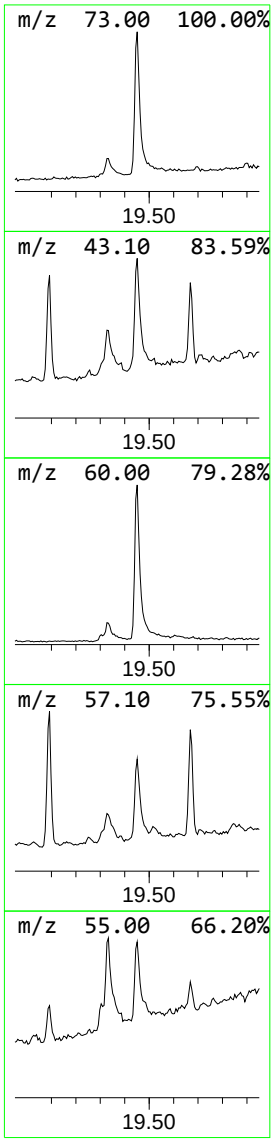
Peak Number 12 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	3.97 ng	954691	Chrysene-d12	21.462

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039397.D
Acq On : 11 Apr 2023 17:21
Operator : CG/JU
Sample : 02262-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-3A-040723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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
2-Pentanone, 4-...	4.952	28.2	ng	1929580	1	7.863	1369110	20.0
Nonadecane	14.410	2.0	ng	258465	3	14.516	2552950	20.0
Hexadecane	15.363	3.4	ng	427161	3	14.516	2552950	20.0
Benzophenone	15.880	2.4	ng	299650	3	14.516	2552950	20.0
Heneicosane	16.221	7.6	ng	1047790	4	17.269	2759890	20.0
Pentadecane	17.021	4.7	ng	651077	4	17.269	2759890	20.0
Hexadecane, 2,6...	17.069	3.4	ng	465514	4	17.269	2759890	20.0
Dodecane, 2-met...	17.763	4.6	ng	633606	4	17.269	2759890	20.0
n-Hexadecanoic ...	18.168	14.9	ng	2053290	4	17.269	2759890	20.0
2-Bromo dodecane	18.457	4.8	ng	658365	4	17.269	2759890	20.0
Eicosane, 10-me...	19.092	2.6	ng	352966	4	17.269	2759890	20.0
Octadecanoic acid	19.451	4.0	ng	954691	5	21.462	4808360	20.0