LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038789.D
Acq On : 20 Feb 2023 16:25
Operator : CG/JU
Sample : 01611-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-17

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-BM020123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038789.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	290	301	309	rBV	256913	355703	9.71%	2.650%
2	5.434	375	382	396	rVB	396377	562612	15.35%	4.191%
3	7.057	651	658	669	rBV	277739	422973	11.54%	3.151%
4	7.875	790	797	804	rVB	147027	226148	6.17%	1.685%
5	9.057	990	998	1005	rBV	365972	577164	15.75%	4.300%
6	10.692	1269	1276	1282	rBV	188384	302062	8.24%	2.250%
7	13.157	1688	1695	1703	rBV	1193269	1627019	44.40%	12.121%
8	13.422	1733	1740	1745	rBV2	31447	47694	1.30%	0.355%
9	14.533	1923	1929	1937	rVB	311054	438411	11.96%	3.266%
10	14.945	1990	1999	2008	rBV	41638	76039	2.07%	0.566%
11	16.027	2177	2183	2190	rBV	1231082	1643927	44.86%	12.247%
12	17.280	2389	2396	2403	rBV	394098	540670	14.75%	4.028%
13	18.174	2538	2548	2559	rBV	287717	472493	12.89%	3.520%
14	18.468	2593	2598	2602	rBV3	25207	39327	1.07%	0.293%
15	18.515	2602	2606	2616	rVB3	29024	50634	1.38%	0.377%
16	19.033	2686	2694	2703	rBV3	52467	134659	3.67%	1.003%
17	19.451	2760	2765	2776	rVB	187844	274312	7.49%	2.044%
18	19.909	2837	2843	2848	rBV	3306646	3664776	100.00%	27.302%
19	20.309	2904	2911	2918	rVB2	57637	137897	3.76%	1.027%
20	21.156	3051	3055	3058	rBV	106606	178263	4.86%	1.328%
21	21.468	3103	3108	3113	rBV	602718	710379	19.38%	5.292%
22	22.009	3196	3200	3205	rVB	85894	135749	3.70%	1.011%
23	23.845	3506	3512	3520	rBV2	446932	804102	21.94%	5.990%

Sum of corrected areas: 13423013

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Instrument :
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ClientSampleId :
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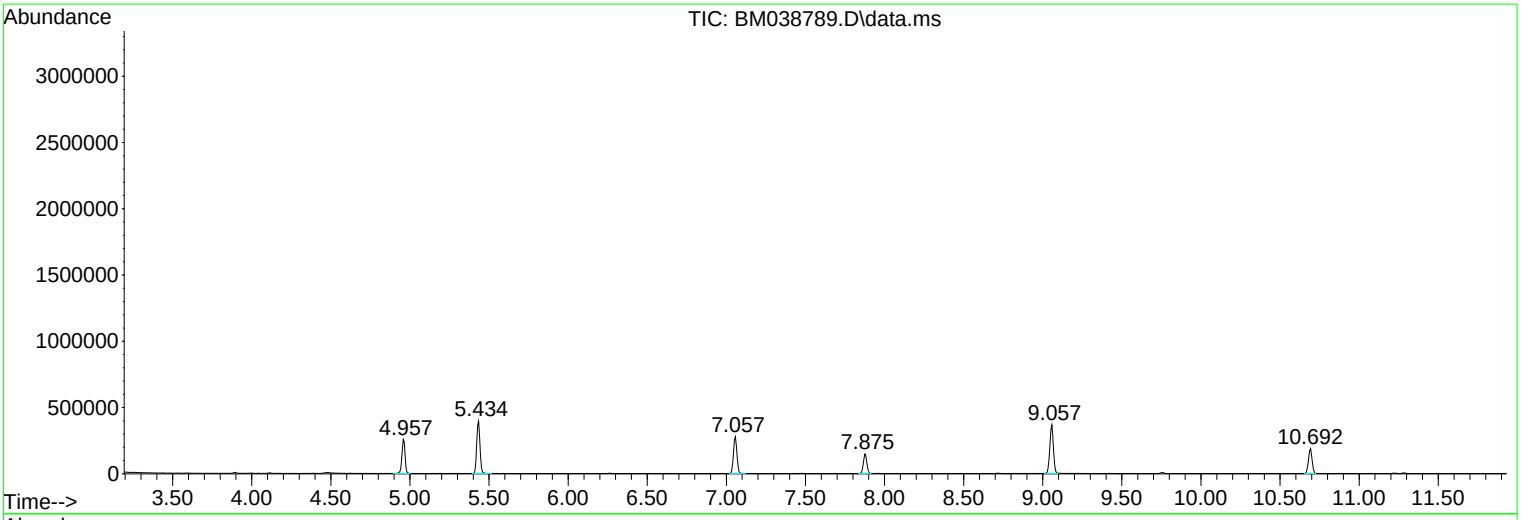
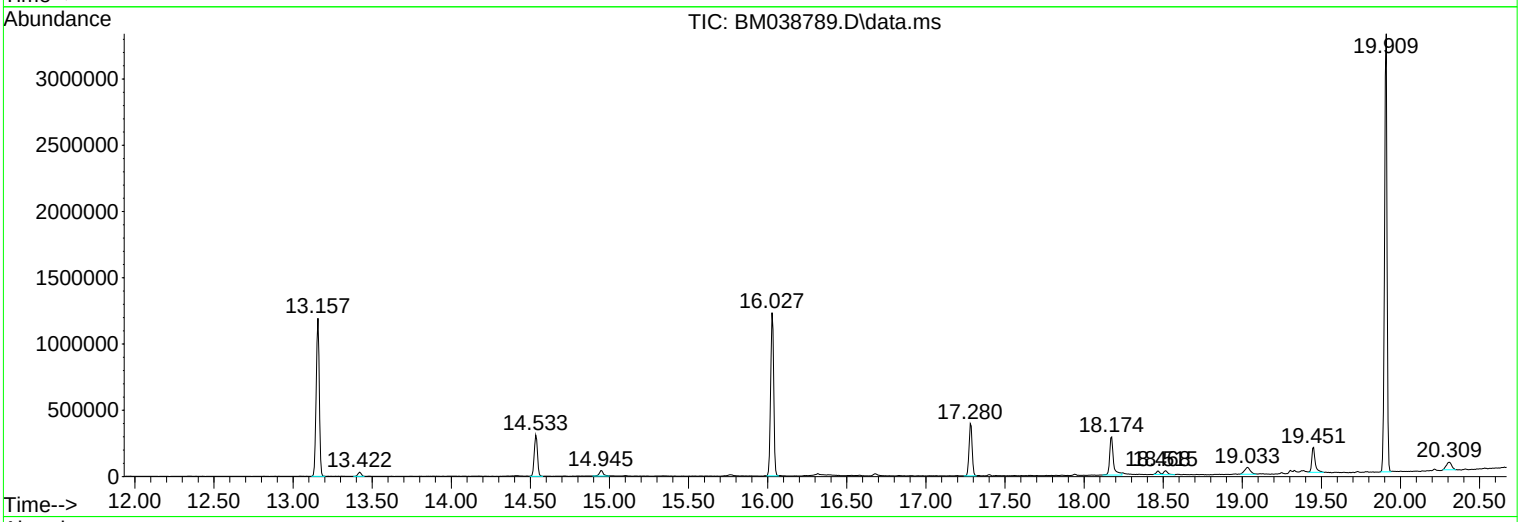
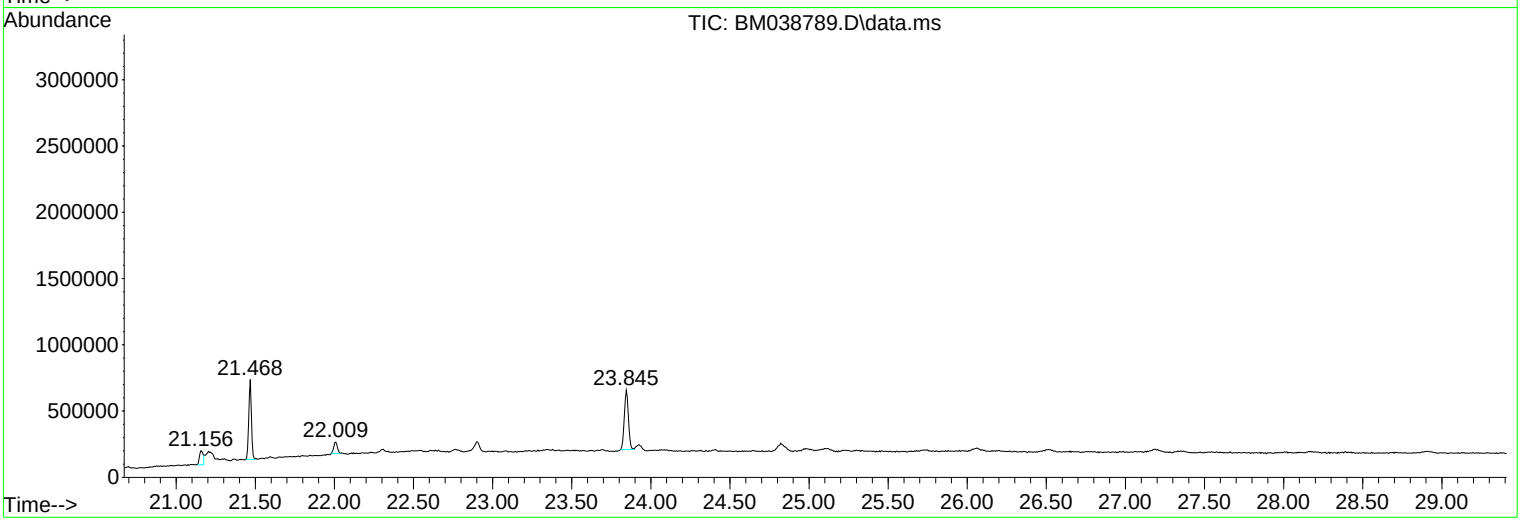
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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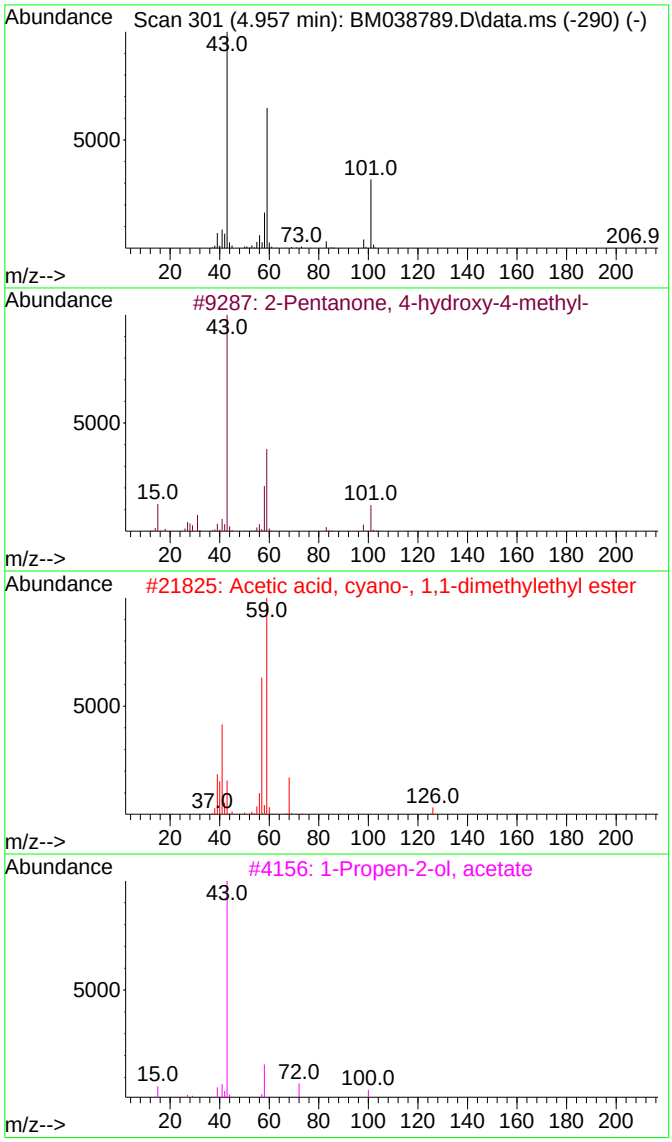
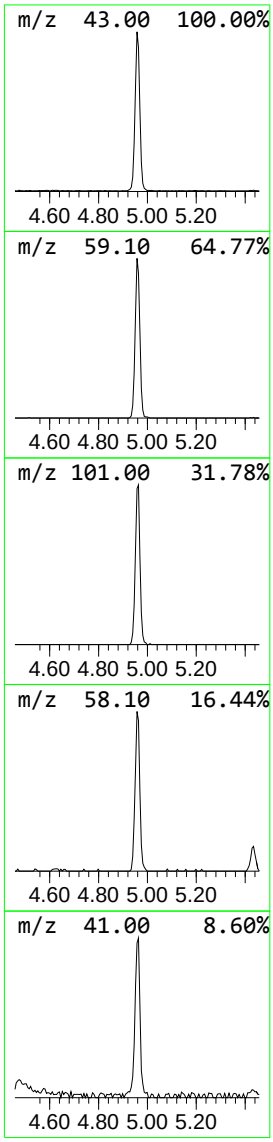
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	31.46 ng	355703	1,4-Dichlorobenzene-d4	7.875

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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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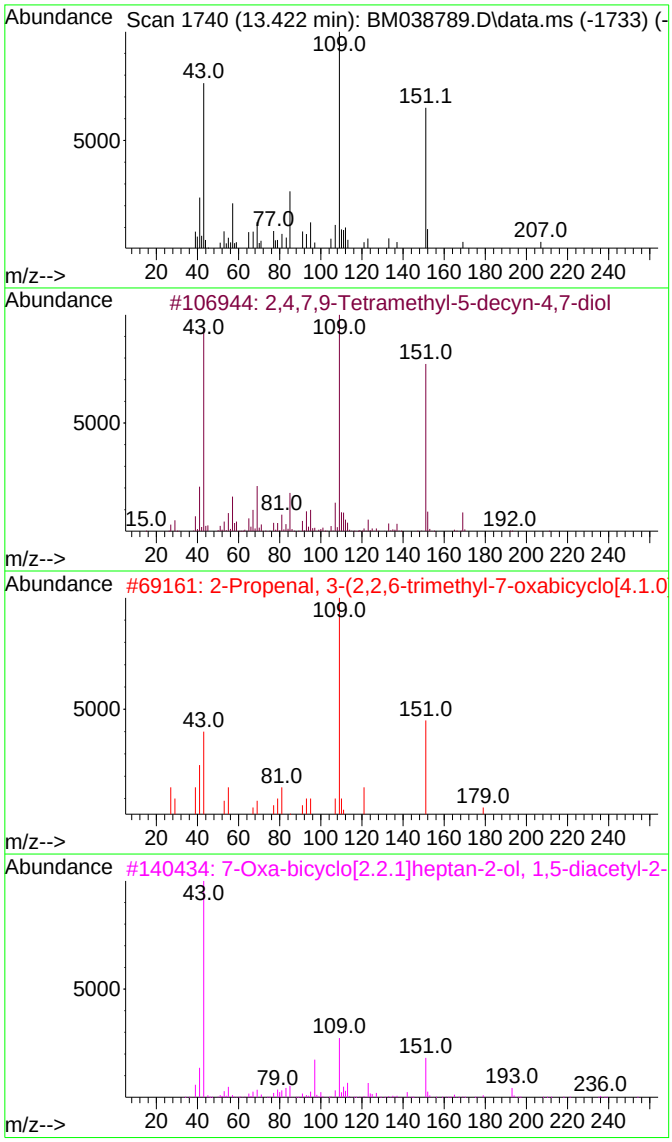
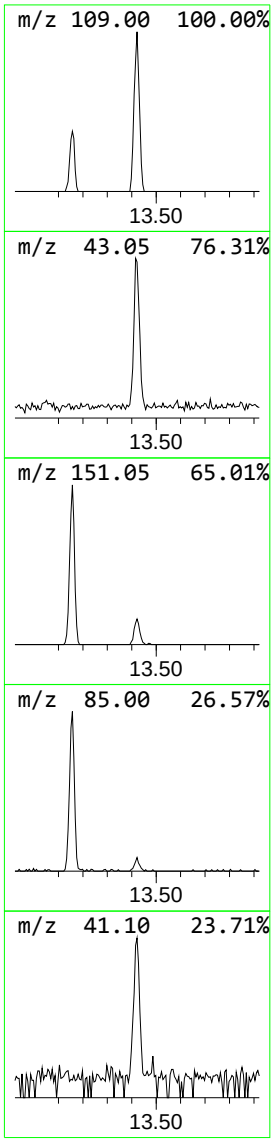
****

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	2.18 ng	47694	Acenaphthene-d10	14.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59
3	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	56
4	N-(4-tert-Butoxyphenyl)acetamide	207	C12H17NO2	002109-73-1	53
5	Metacetamol	151	C8H9NO2	000621-42-1	53





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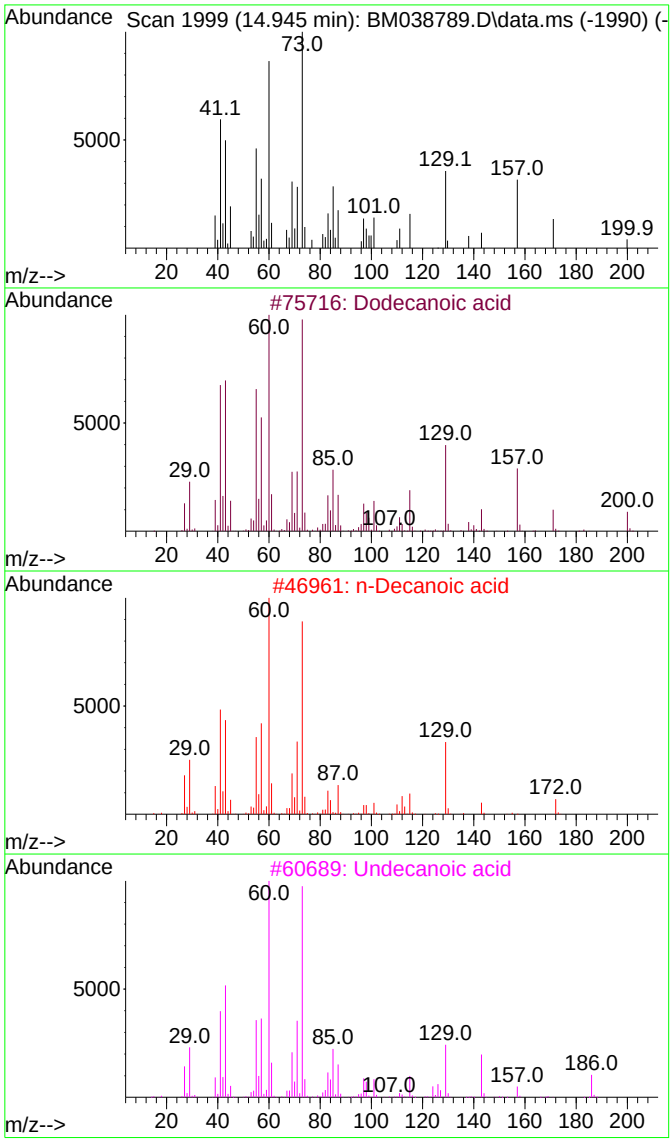
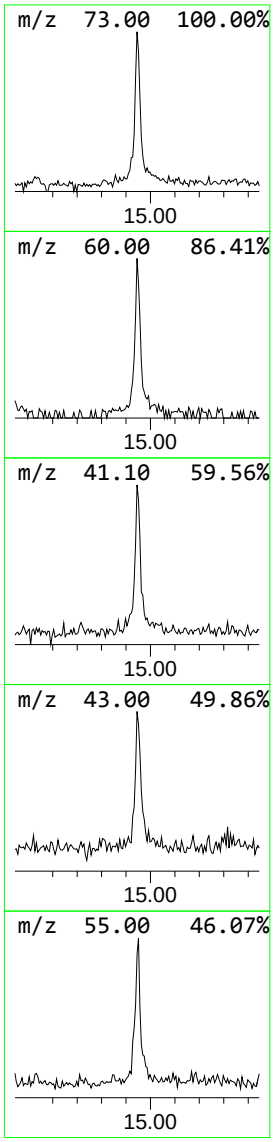
****

Peak Number 3 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.945	3.47 ng	76039	Acenaphthene-d10	14.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	93
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	Undecanoic acid	186	C11H22O2	000112-37-8	50
4	Nonanoic acid	158	C9H18O2	000112-05-0	47
5	Benzamide, 4-butoxy-N-[2-(2-thie...	303	C17H21NO2S	1000319-87-5	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

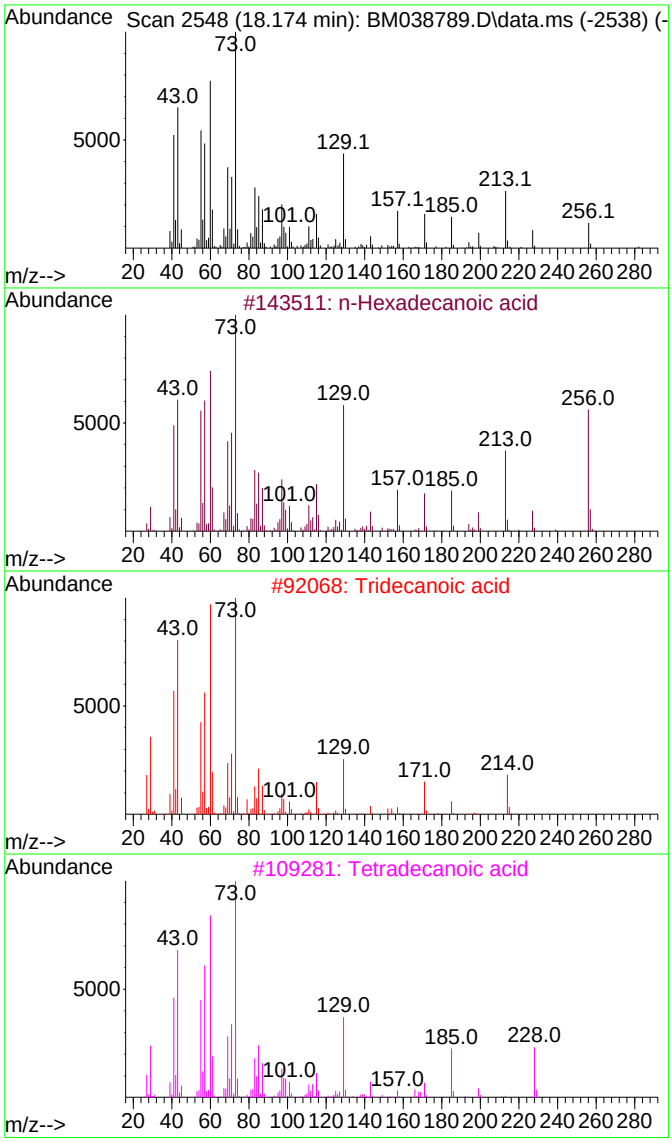
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

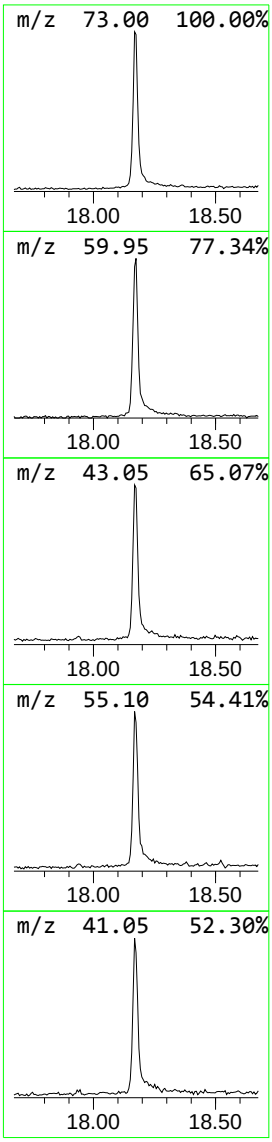
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	17.48 ng	472493	Phenanthrene-d10	17.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49





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Instrument :
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ClientSampleId :
EB-2023-2-17

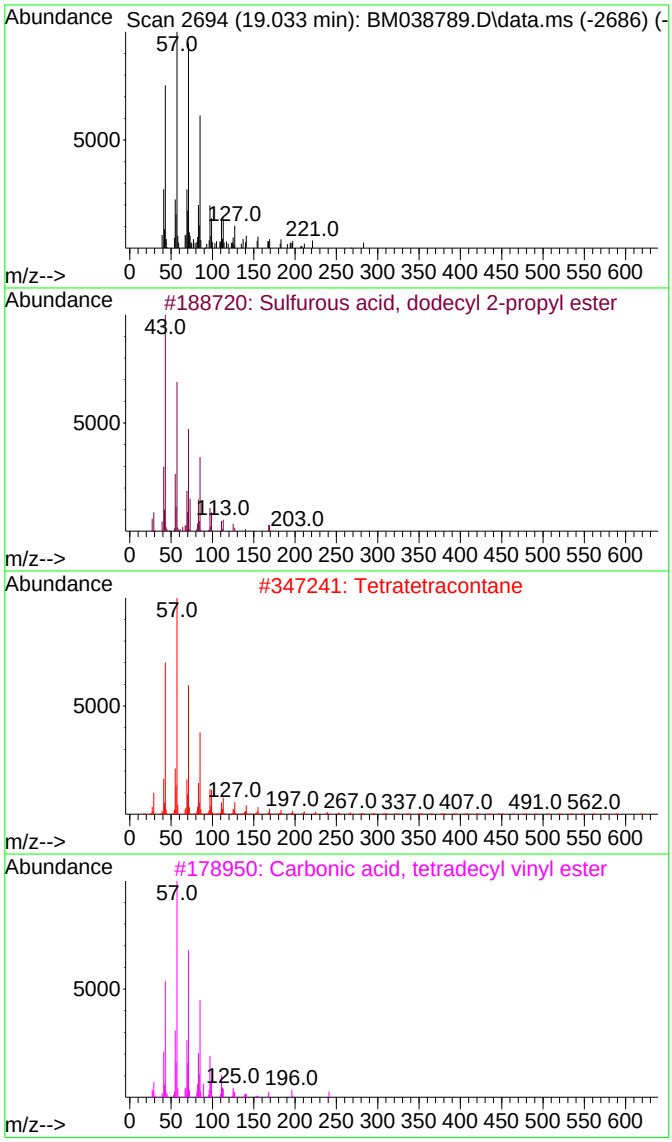
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

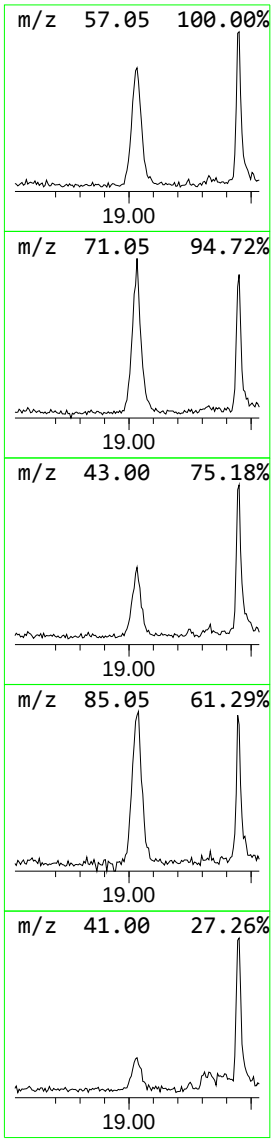
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Sulfurous acid, dodecyl 2-p... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.033	4.98 ng	134659	Phenanthrene-d10	17.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
5	Eicosane	282	C20H42	000112-95-8	80





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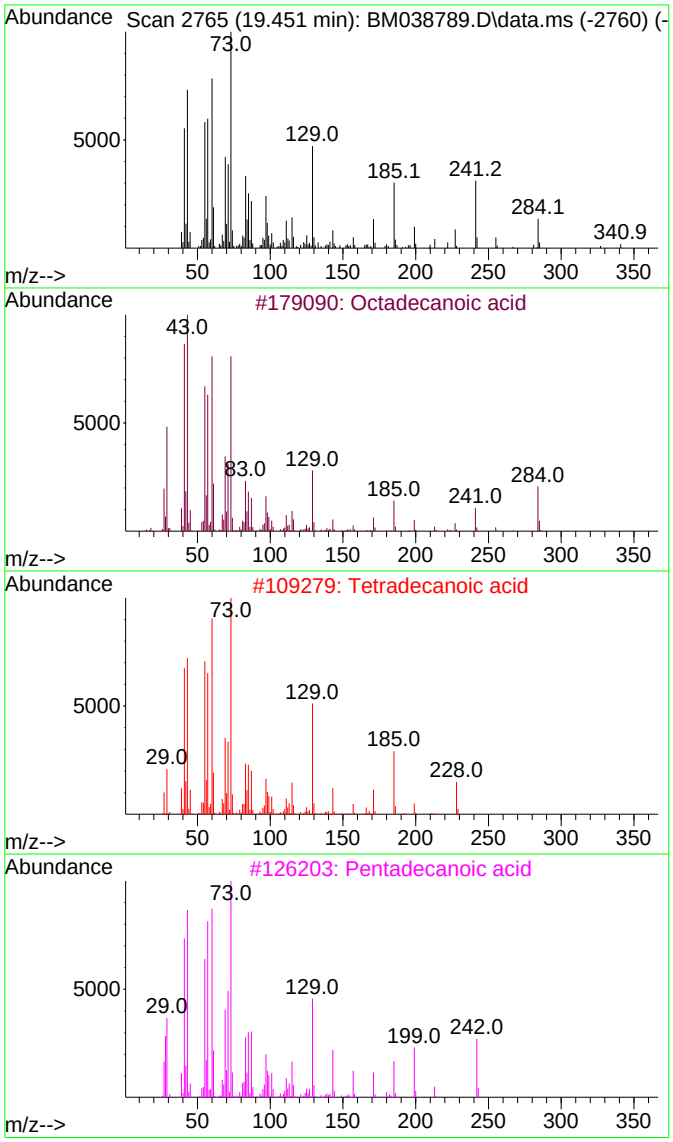
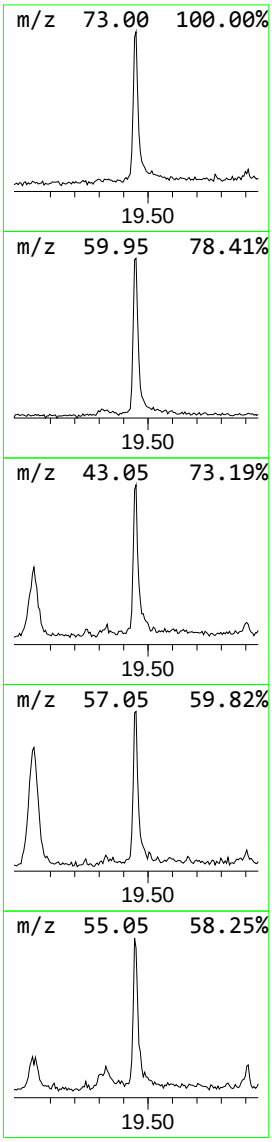
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	7.72 ng	274312	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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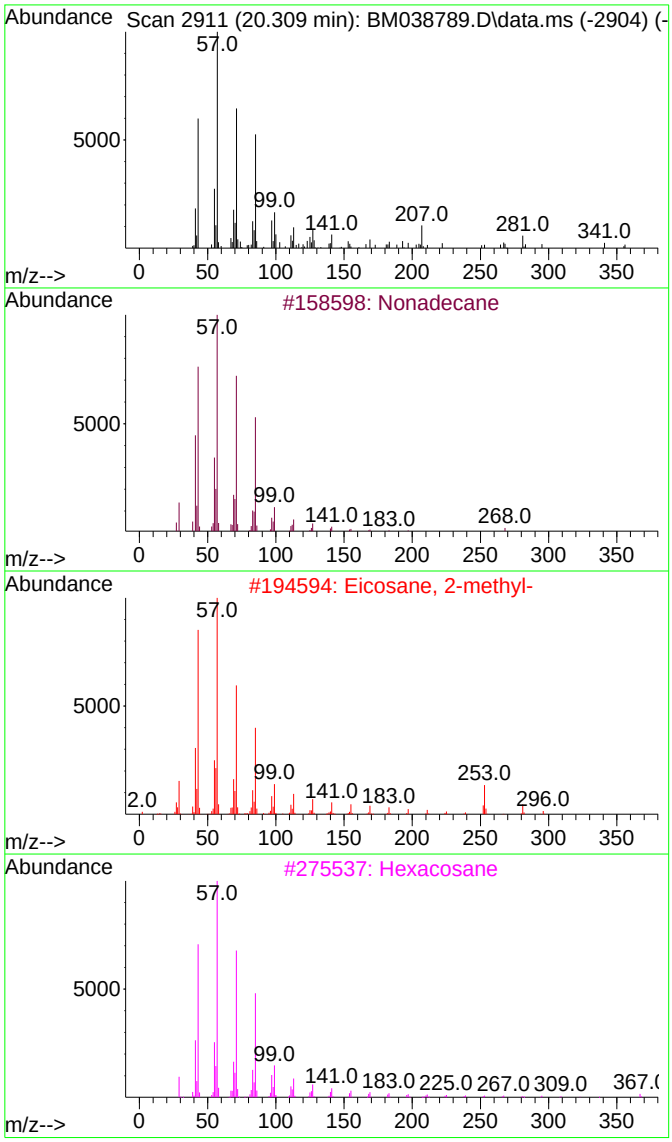
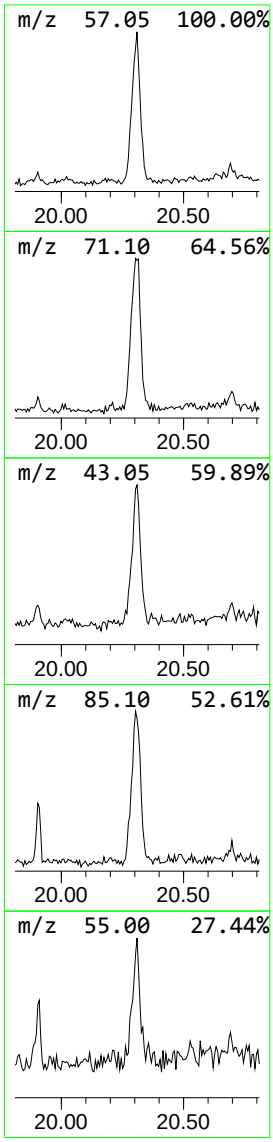
****

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.309	3.88 ng	137897	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5	4-Methylheneicosane	310	C22H46	025117-29-7	83





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TIC Library : C:\Database\NIST20.L
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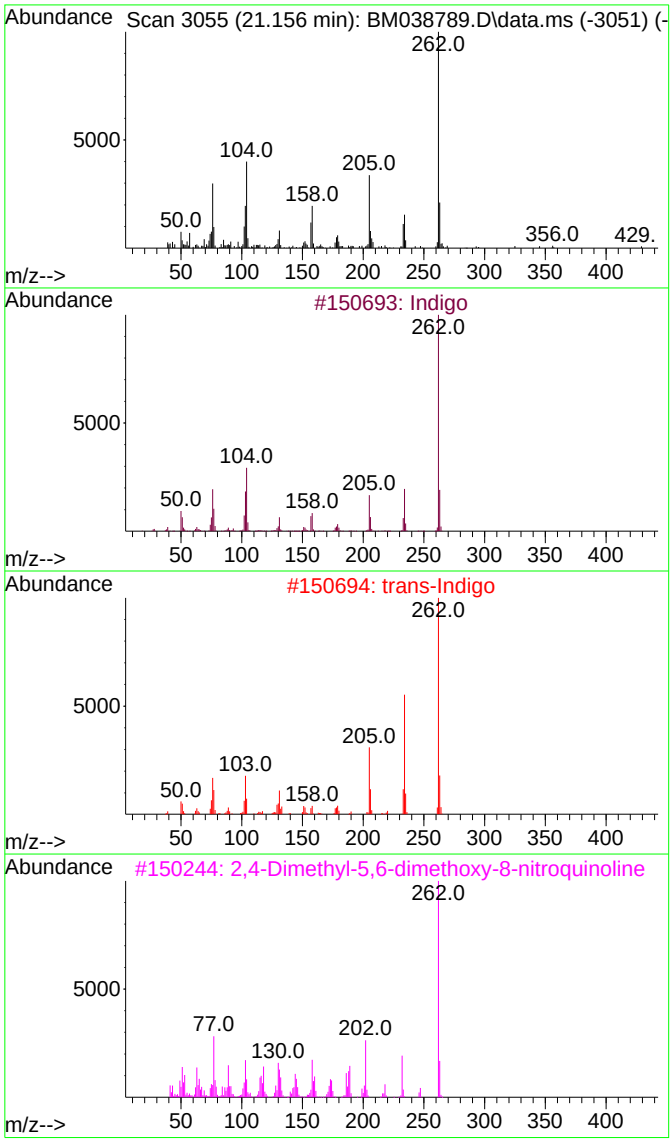
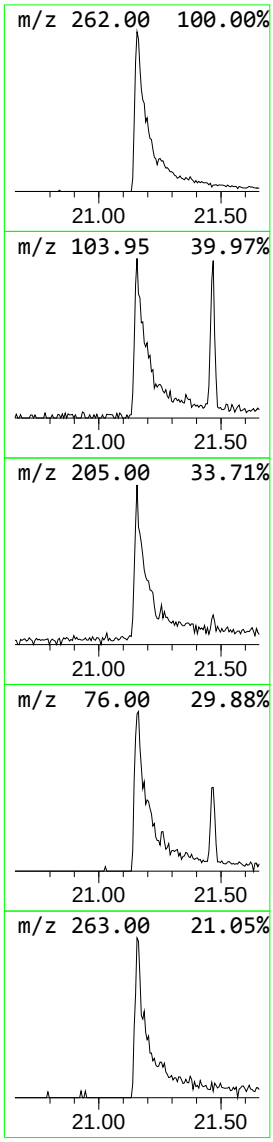
****

Peak Number 8 Indigo Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	5.02 ng	178263	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indigo	262	C16H10N2O2	000482-89-3	96
2	trans-Indigo	262	C16H10N2O2	064784-13-0	50
3	2,4-Dimethyl-5,6-dimethoxy-8-nit...	262	C13H14N2O4	082082-03-9	47
4	Lanceolatin B	262	C17H10O3	000482-00-8	43
5	1,2,3,6,7,8,9,10,11,12-Decahydro...	262	C20H22	092387-50-3	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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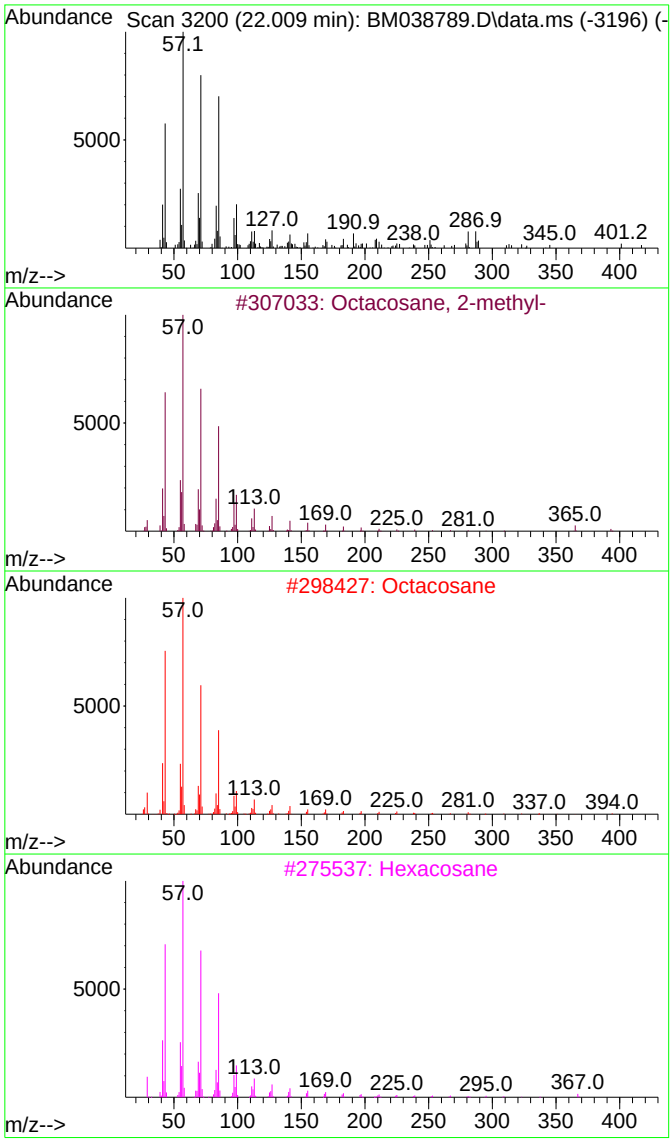
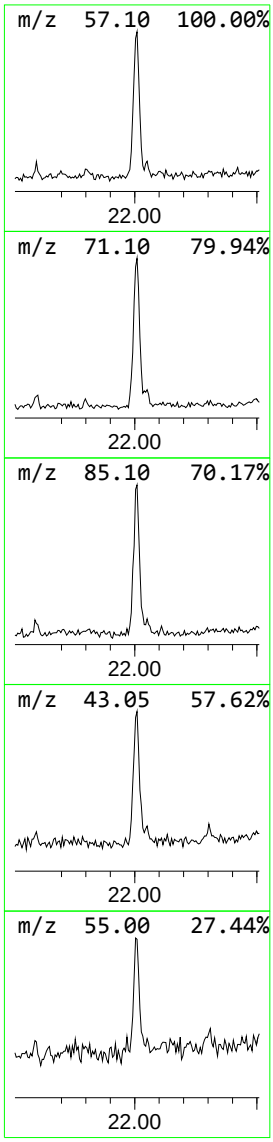
****

Peak Number 9 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.009	3.82 ng	135749	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	74
2	Octacosane	394	C28H58	000630-02-4	74
3	Hexacosane	366	C26H54	000630-01-3	74
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	72





Tentatively Identified Compound (LSC) summary

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Sample : 01611-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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-...	4.957	31.5	ng	355703	1	7.875	226148	20.0
2,4,7,9-Tetrame...	13.422	2.2	ng	47694	3	14.533	438411	20.0
Dodecanoic acid	14.945	3.5	ng	76039	3	14.533	438411	20.0
n-Hexadecanoic ...	18.174	17.5	ng	472493	4	17.280	540670	20.0
Sulfurous acid,...	19.033	5.0	ng	134659	4	17.280	540670	20.0
Octadecanoic acid	19.451	7.7	ng	274312	5	21.468	710379	20.0
Nonadecane	20.309	3.9	ng	137897	5	21.468	710379	20.0
Indigo	21.156	5.0	ng	178263	5	21.468	710379	20.0
Octacosane, 2-m...	22.009	3.8	ng	135749	5	21.468	710379	20.0