LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046707.D
Acq On : 18 Jul 2024 18:01
Operator : MA/JU
Sample : P3248-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-120-SB02

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-BM071724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046707.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	60	64	71	rBV	48766	61073	2.21%	0.332%
2	4.687	281	289	296	rBV	63590	91408	3.31%	0.496%
3	5.134	358	365	373	rBV	1155257	1582779	57.30%	8.596%
4	6.687	623	629	638	rVB	1099516	1664308	60.25%	9.039%
5	7.487	758	765	773	rVB	334988	499873	18.10%	2.715%
6	8.628	952	959	967	rBV	680226	1058491	38.32%	5.749%
7	10.245	1227	1234	1242	rVB	364629	593049	21.47%	3.221%
8	10.998	1356	1362	1371	rBV3	25808	49245	1.78%	0.267%
9	12.745	1652	1659	1666	rBV	1664682	2426531	87.85%	13.179%
10	14.133	1889	1895	1901	rBV	527748	737715	26.71%	4.007%
11	14.674	1979	1987	2033	rBV	165216	908978	32.91%	4.937%
12	15.633	2139	2150	2158	rBV	1406025	1943552	70.36%	10.556%
13	16.886	2357	2363	2369	rVB	583294	787773	28.52%	4.279%
14	17.821	2516	2522	2531	rBV	243150	366943	13.28%	1.993%
15	19.115	2738	2742	2749	rBV3	102318	139117	5.04%	0.756%
16	19.545	2809	2815	2820	rBV	2227419	2762138	100.00%	15.002%
17	20.556	2983	2987	2993	rBV	186321	202906	7.35%	1.102%
18	20.850	3033	3037	3044	rBV	267912	349853	12.67%	1.900%
19	21.115	3077	3082	3087	rVB	638962	818579	29.64%	4.446%
20	21.550	3152	3156	3162	rVB3	142832	191183	6.92%	1.038%
21	22.768	3359	3363	3369	rVB3	110208	180894	6.55%	0.982%
22	23.880	3545	3552	3562	rVB2	433793	995929	36.06%	5.409%

Sum of corrected areas: 18412317

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
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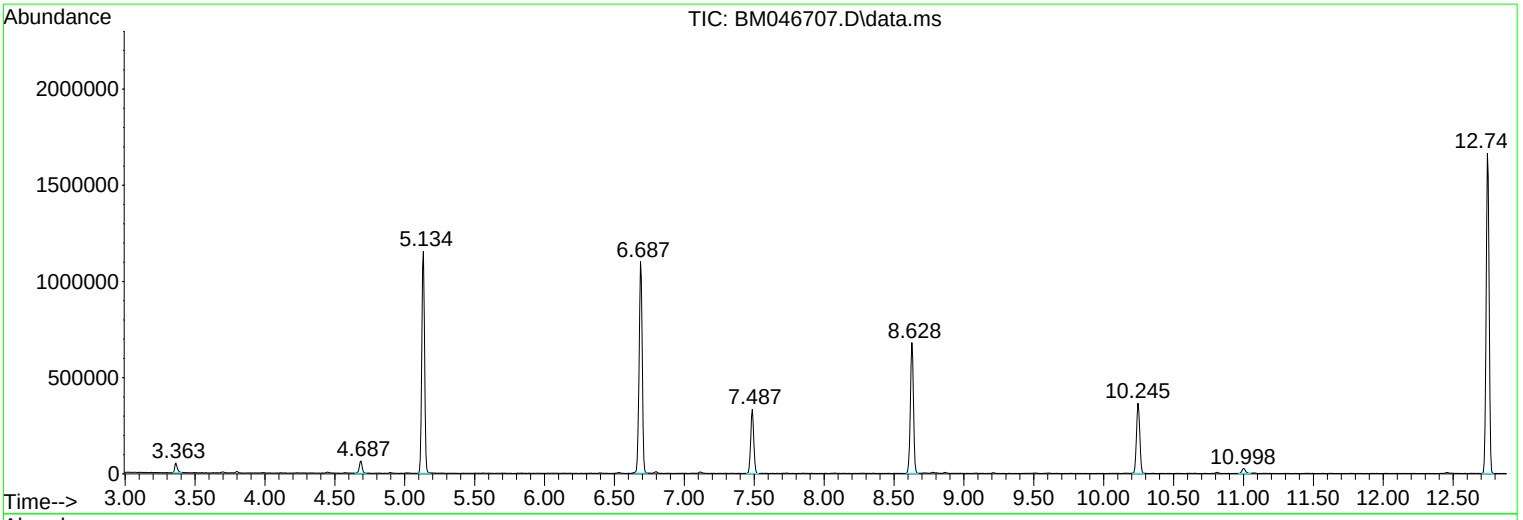
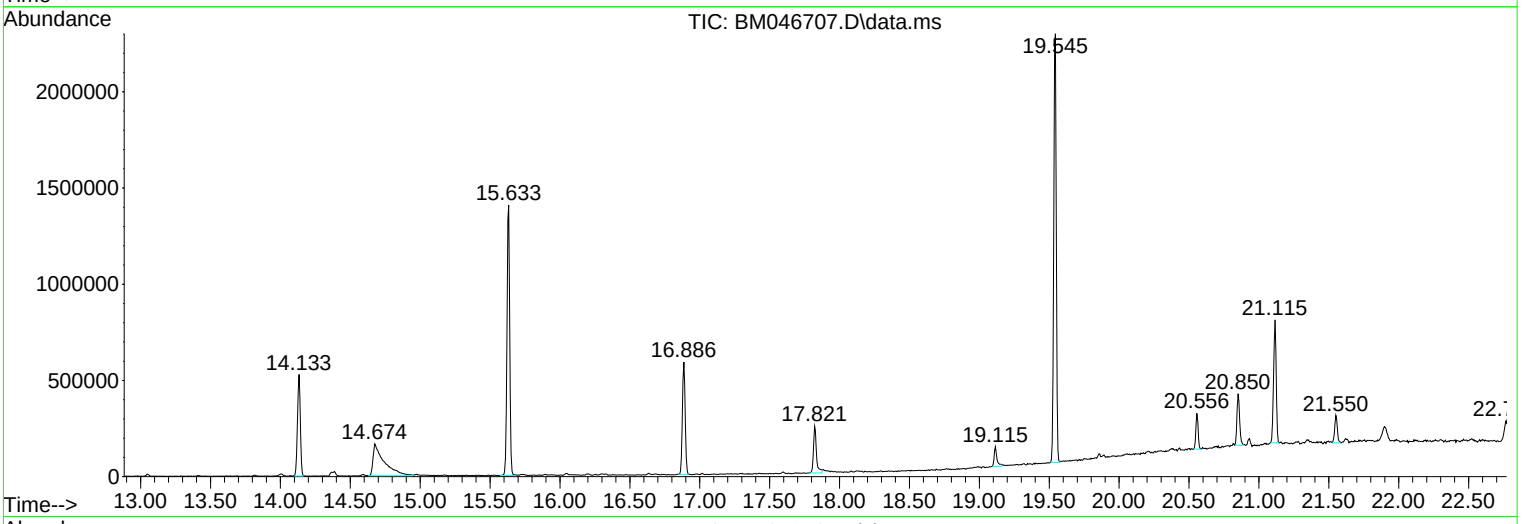
ALS Vial : 8 Sample Multiplier: 1

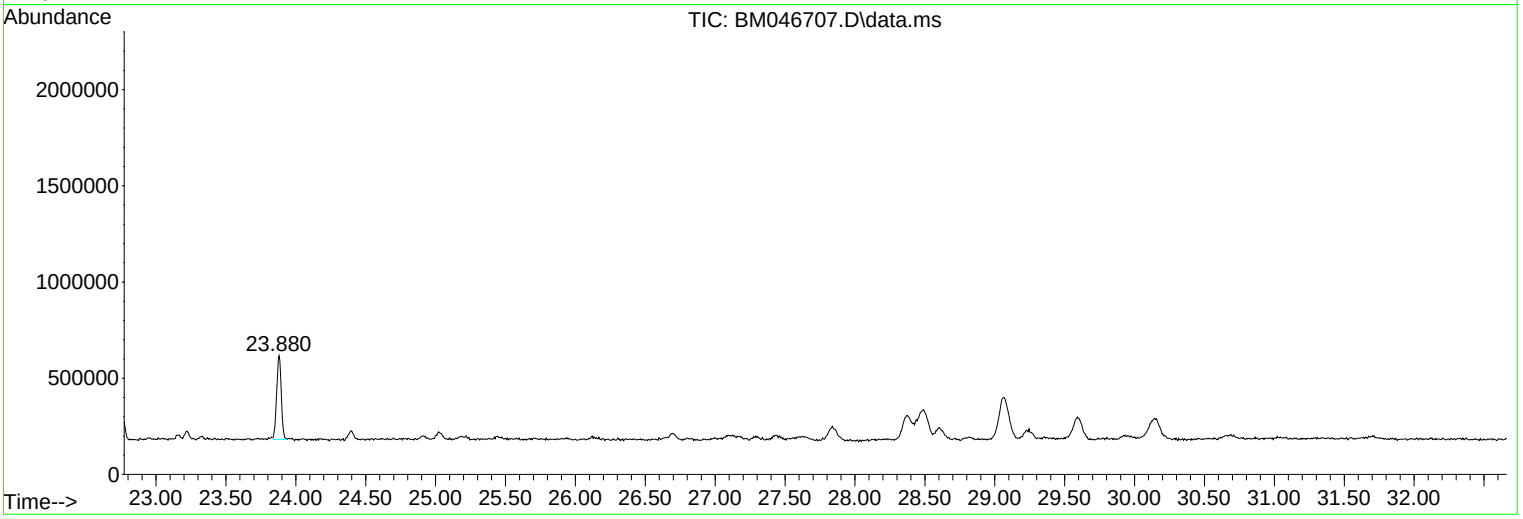
Instrument :
BNA_M
ClientSampleId :
B-120-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.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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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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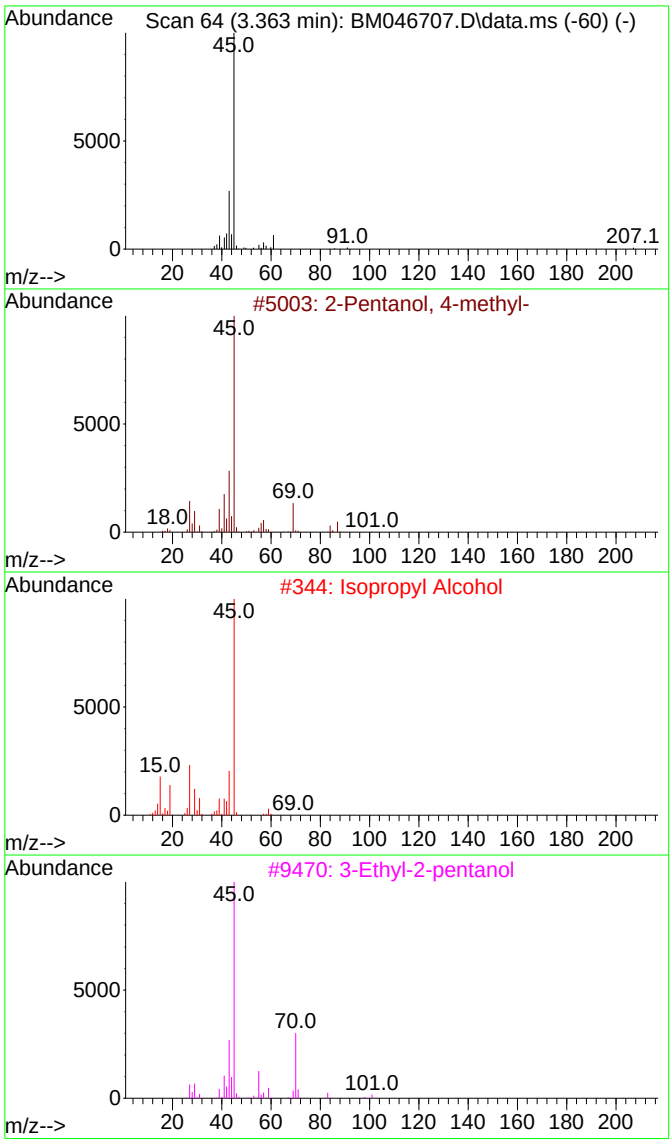
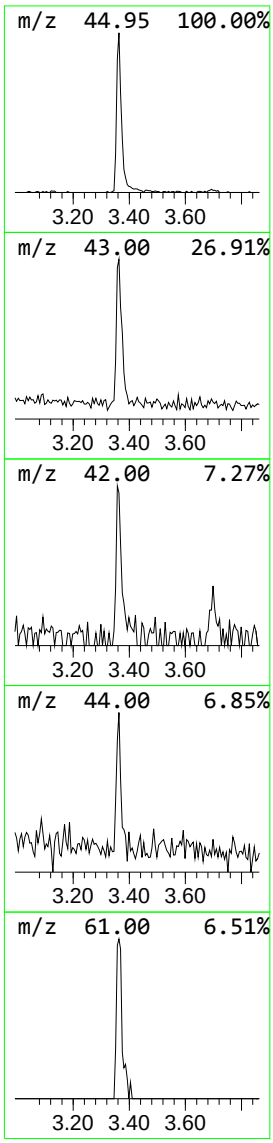
Peak Number 1 unknown3.363 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	2.44 ng	61073	1,4-Dichlorobenzene-d4	7.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	39
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9
4	2-Heptanol	116	C7H16O	000543-49-7	9
5	2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9





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TIC Library : C:\Database\NIST20.L
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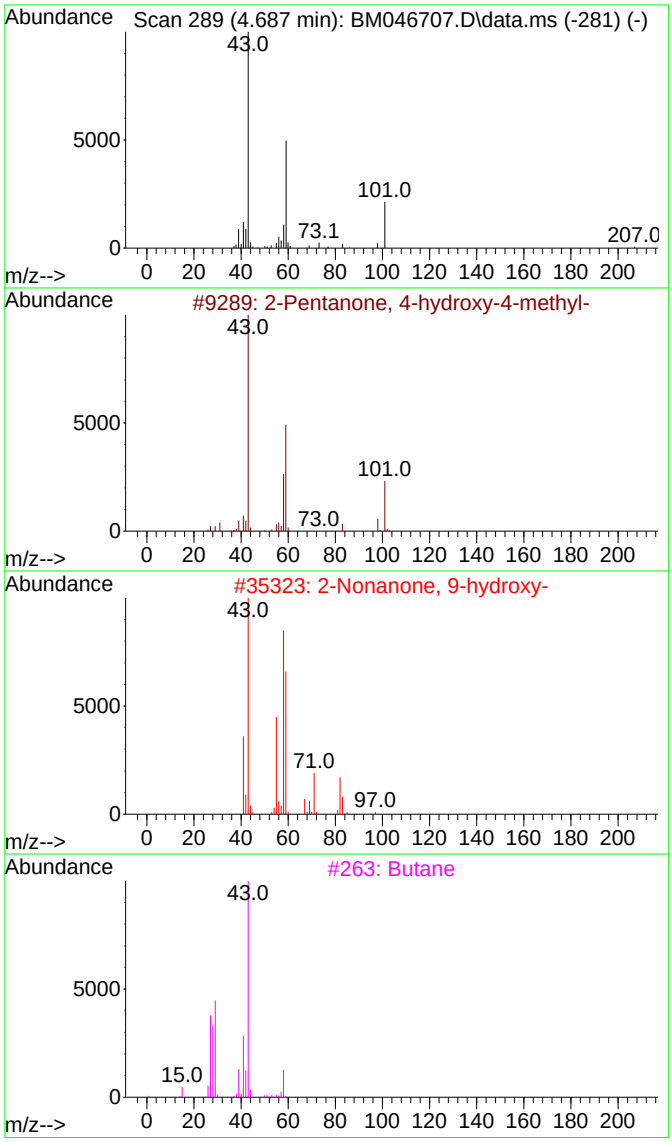
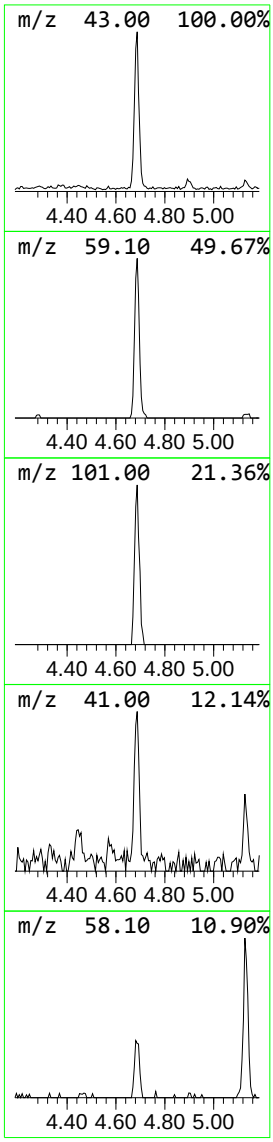
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	3.66 ng	91408	1,4-Dichlorobenzene-d4	7.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	Butane	58	C4H10	000106-97-8	14
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propylamine	59	C3H9N	000107-10-8	9





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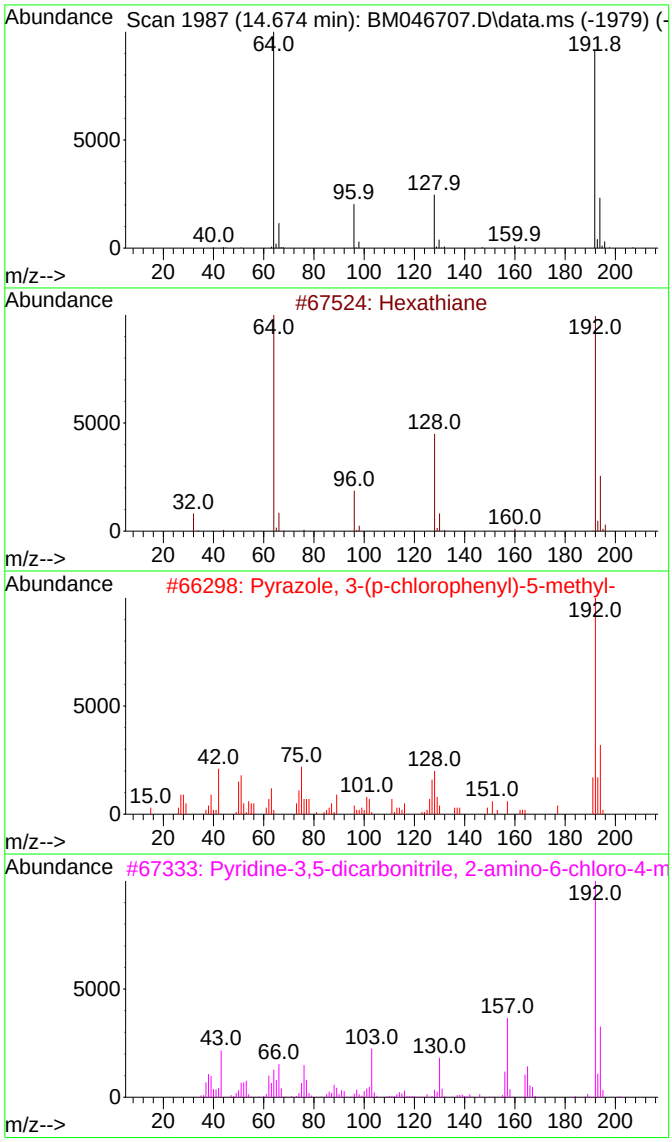
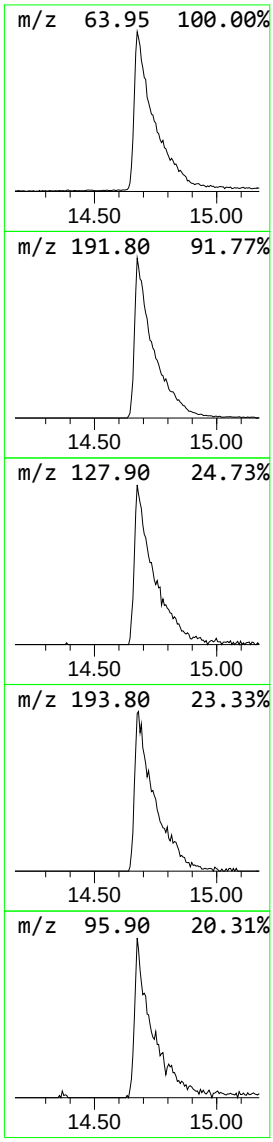
Peak Number 3 Hexathiane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	24.64 ng	908978	Acenaphthene-d10	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	9
3	Pyridine-3,5-dicarbonitrile, 2-a...	192	C8H5ClN4	064829-09-0	9
4	1,2-Phenylene diisothiocyanate	192	C8H4N2S2	071105-17-4	9
5	Valine, N-methyl-N-(2-chloroetho...	447	C24H46ClNO4	1000328-89-3	9





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Sample : P3248-02
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
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TIC Library : C:\Database\NIST20.L
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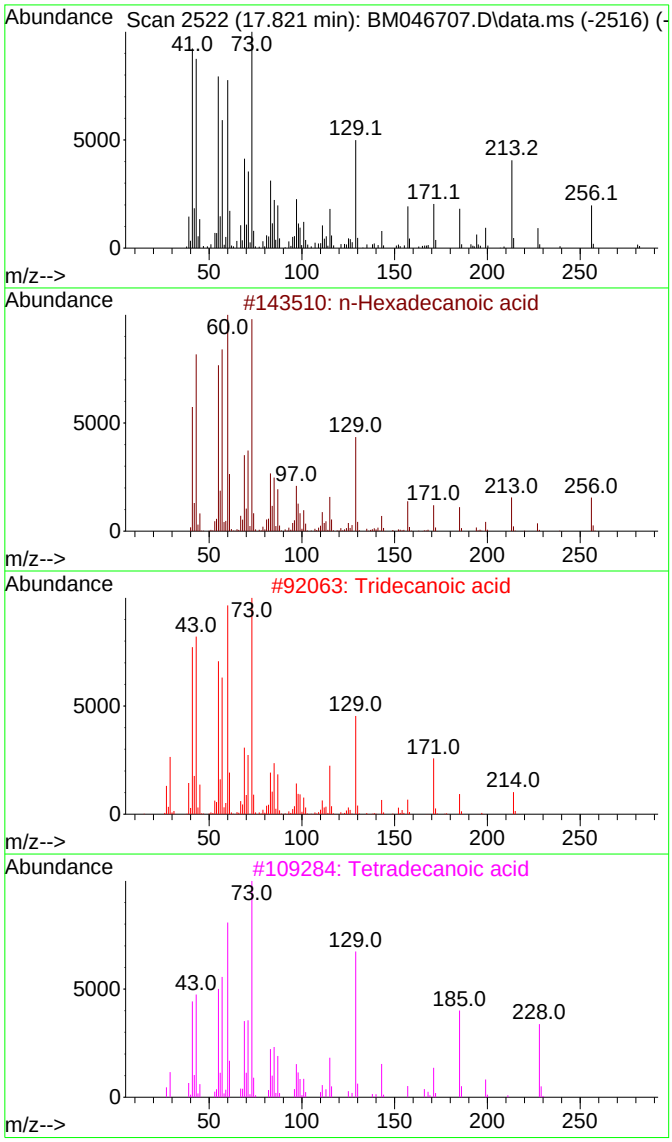
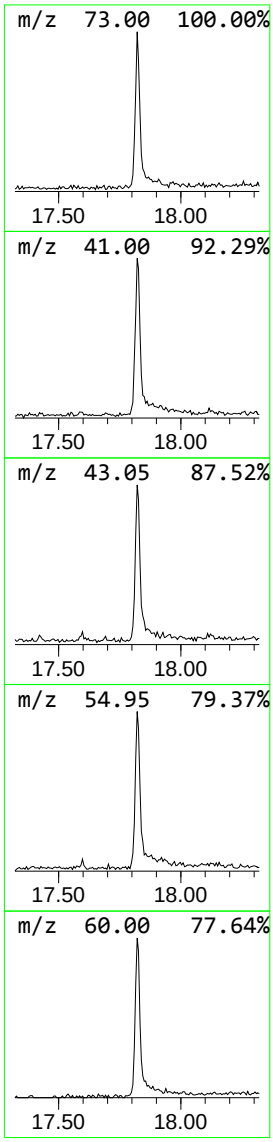
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	9.32 ng	366943	Phenanthrene-d10	16.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Operator : MA/JU
Sample : P3248-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-120-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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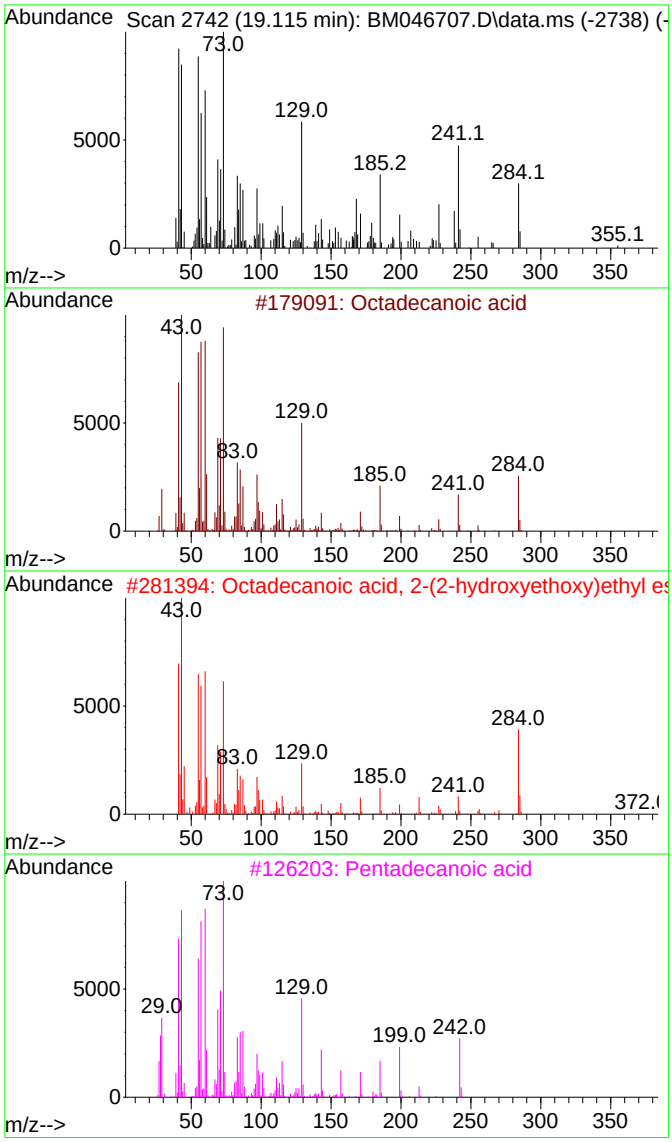
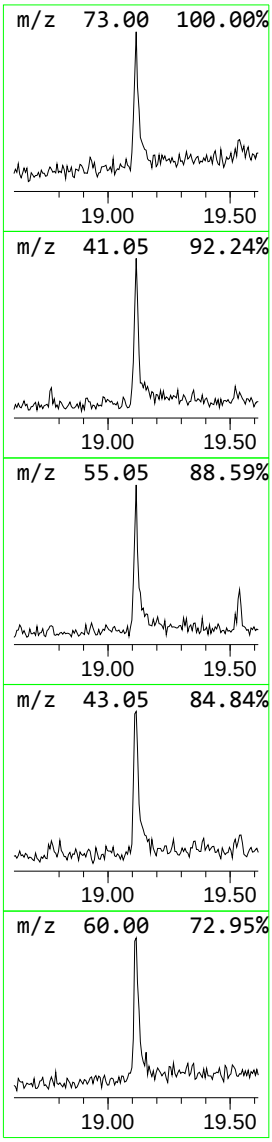
Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.115	3.40 ng	139117	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Undecanoic acid	186	C11H22O2	000112-37-8	25





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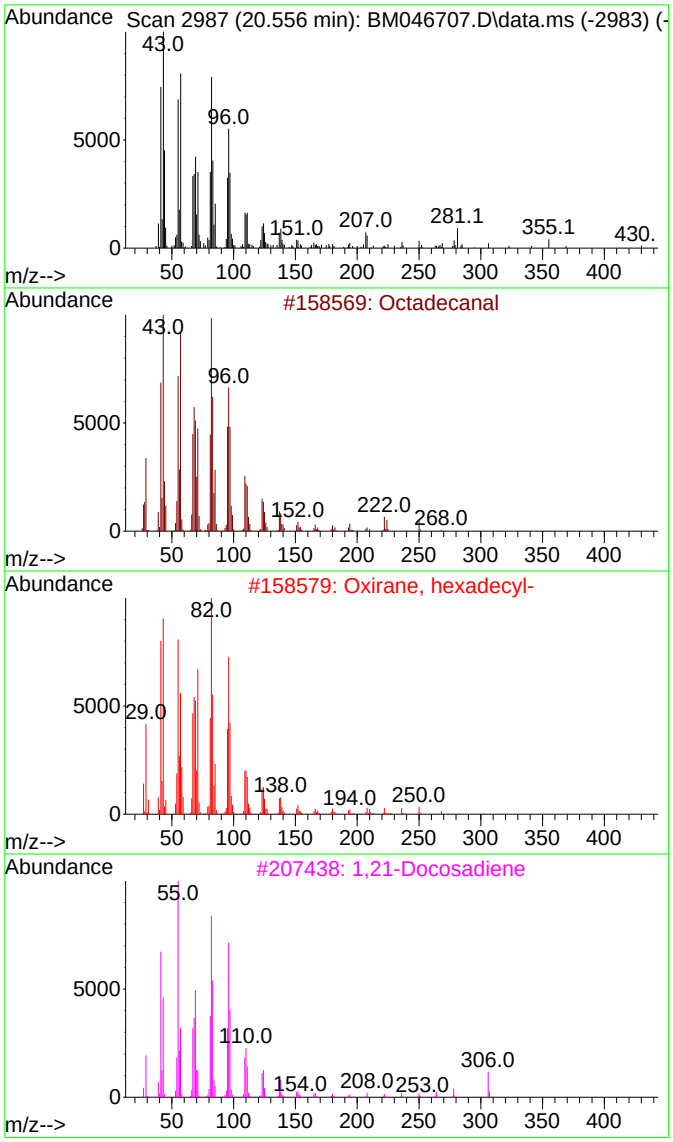
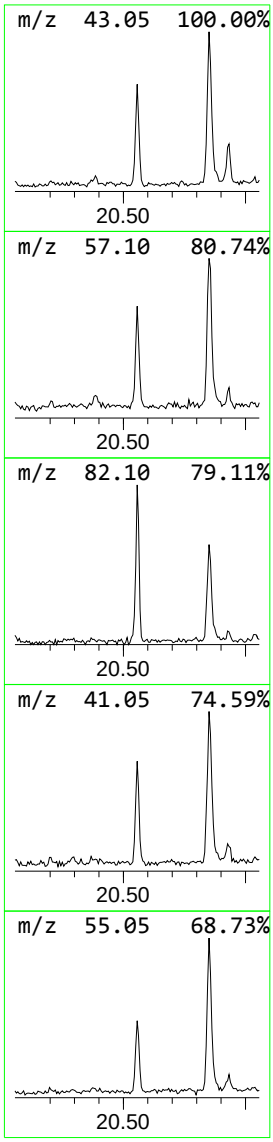
Peak Number 6 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.556	4.96 ng	202906	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
3	1,21-Docosadiene	306	C22H42	053057-53-7	95
4	14-Heptadecenal	252	C17H32O	1010144-58-0	91
5	Docosanal	324	C22H44O	057402-36-5	90





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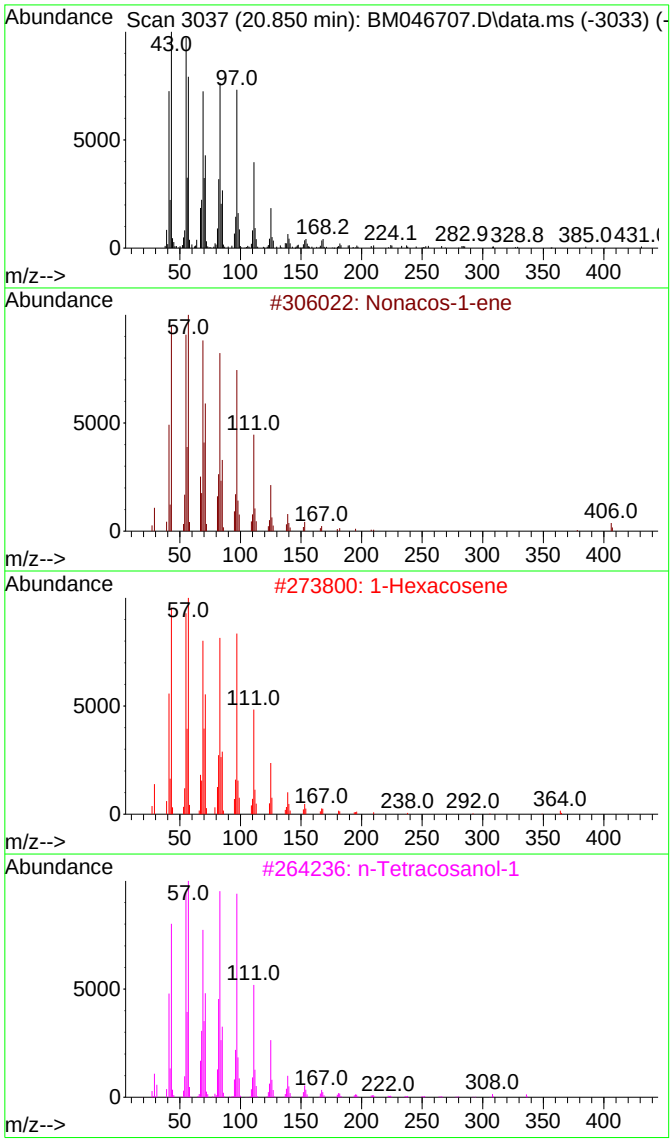
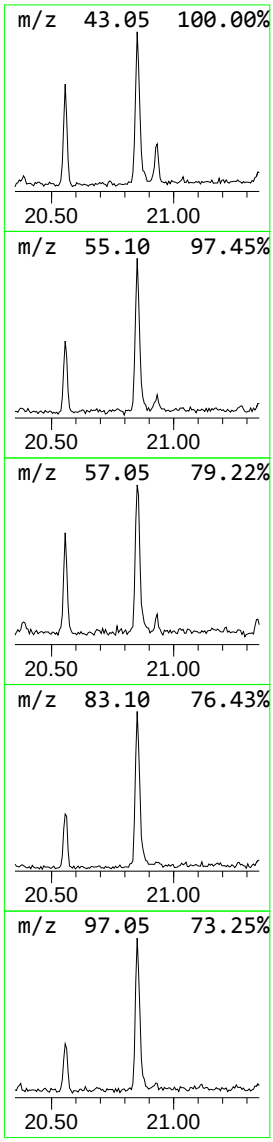
Peak Number 7 Nonacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.850	8.55 ng	349853	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	95
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





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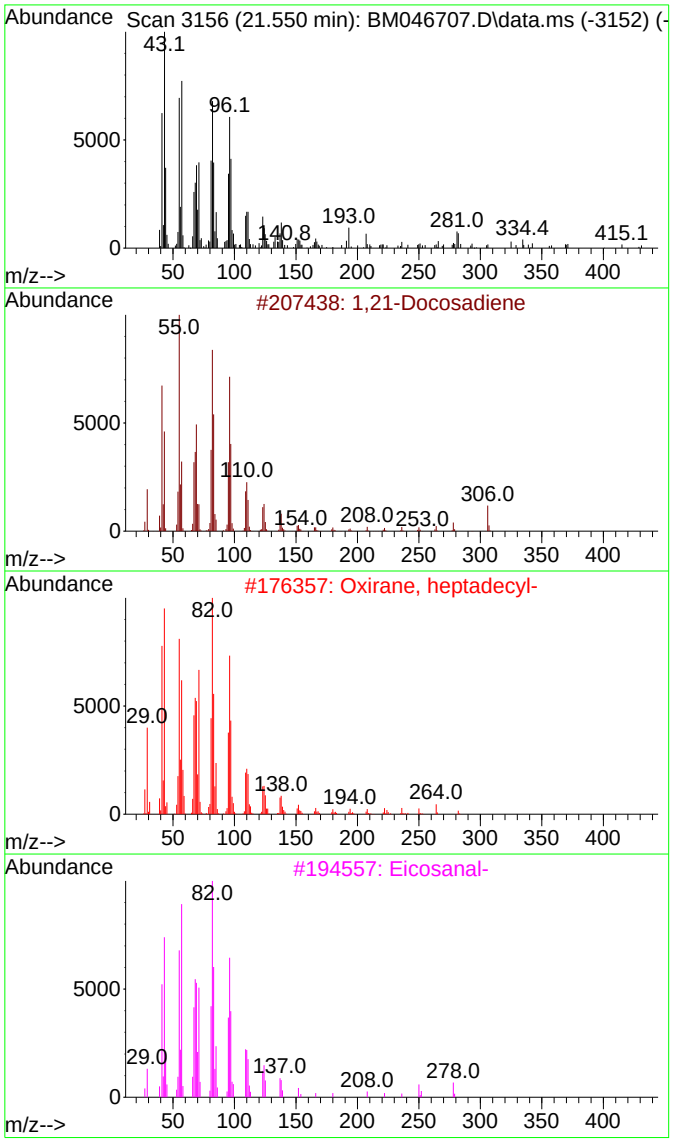
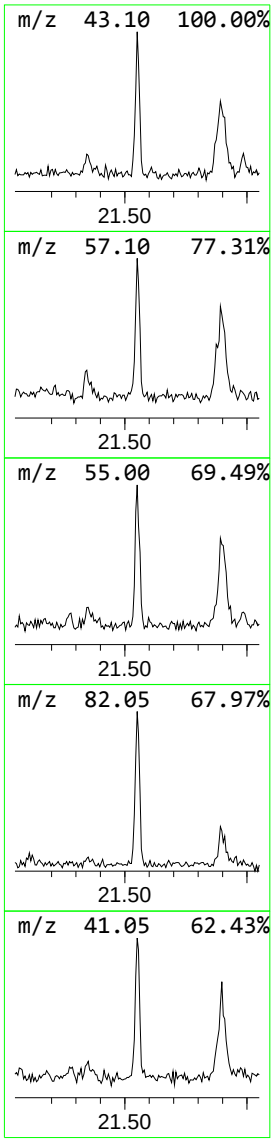
Peak Number 8 1,21-Docosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.550	4.67 ng	191183	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	97
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
3	Eicosanal-	296	C20H40O	002400-66-0	68
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68
5	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	68





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TIC Library : C:\Database\NIST20.L
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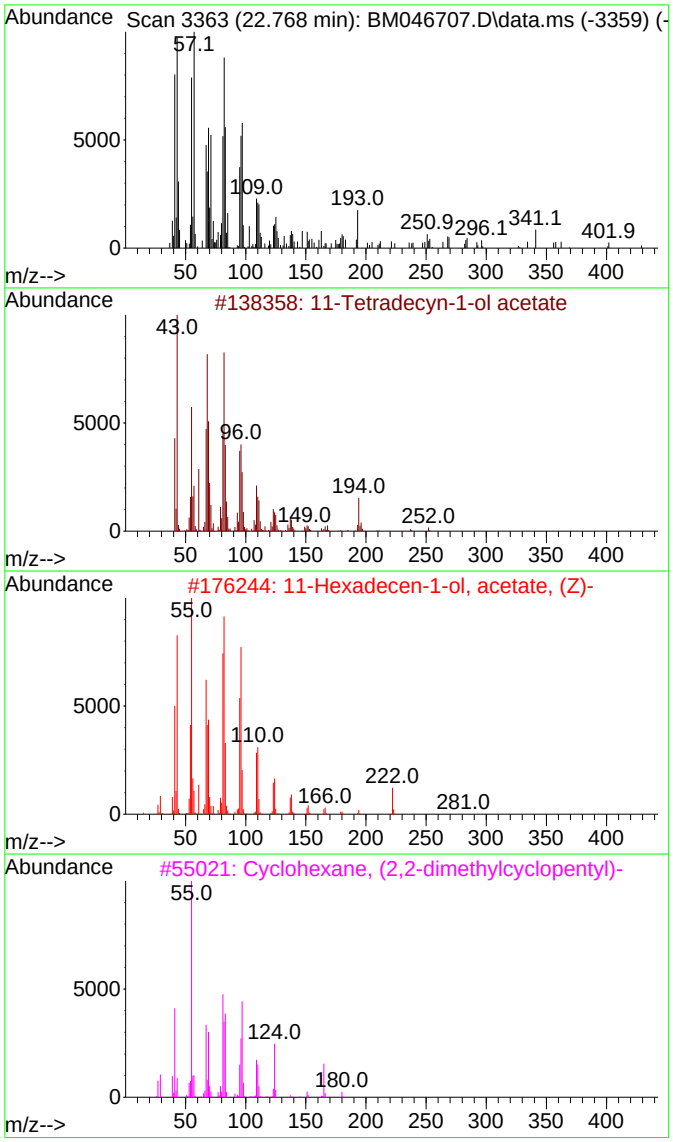
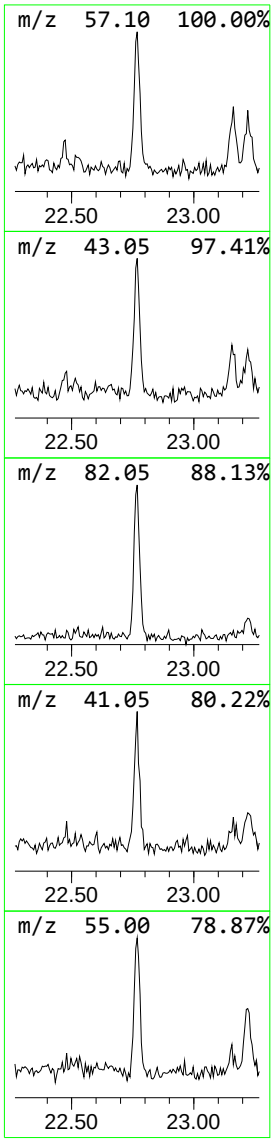
Peak Number 9 11-Tetradecyn-1-ol acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.768	3.63 ng	180894	Perylene-d12	23.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	93
2	11-Hexadecen-1-ol, acetate, (Z)-	282	C18H34O2	034010-21-4	70
3	Cyclohexane, (2,2-dimethylcyclop...	180	C13H24	061142-23-2	70
4	9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	62
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	58





Tentatively Identified Compound (LSC) summary

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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
unknown3.363	3.363	2.4	ng	61073	1	7.487	499873	20.0
2-Pentanone, 4-...	4.687	3.7	ng	91408	1	7.487	499873	20.0
Hexathiane	14.674	24.6	ng	908978	3	14.133	737715	20.0
n-Hexadecanoic ...	17.821	9.3	ng	366943	4	16.886	787773	20.0
Octadecanoic acid	19.115	3.4	ng	139117	5	21.115	818579	20.0
Octadecanal	20.556	5.0	ng	202906	5	21.115	818579	20.0
Nonacos-1-ene	20.850	8.6	ng	349853	5	21.115	818579	20.0
1,21-Docosadiene	21.550	4.7	ng	191183	5	21.115	818579	20.0
11-Tetradecyn-1...	22.768	3.6	ng	180894	6	23.880	995929	20.0