LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111121\
Data File : BF126124.D
Acq On : 11 Nov 2021 13:45
Operator : JU/CG
Sample : M4576-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1

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_F\METHODS\8270-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	497	501	508	rVB	223669	215394	3.60%	0.767%
2	5.445	567	571	575	rBV	1293388	1210030	20.22%	4.309%
3	6.463	740	744	751	rVB	844278	755403	12.62%	2.690%
4	6.839	805	808	812	rBV	1022964	784307	13.11%	2.793%
5	6.981	828	832	838	rBV	416611	359044	6.00%	1.279%
6	7.404	899	904	907	rBV	3055743	2672311	44.66%	9.516%
7	8.122	1023	1026	1030	rBV	1153919	1012621	16.92%	3.606%
8	9.204	1205	1210	1213	rBV	5511189	4762073	79.58%	16.957%
9	9.880	1320	1325	1328	rBV	1483129	1287217	21.51%	4.584%
10	10.669	1454	1459	1462	rBV	2640570	2504465	41.85%	8.918%
11	11.363	1574	1577	1581	rVB	1651243	1329463	22.22%	4.734%
12	11.757	1640	1644	1647	rBV	1528292	1286497	21.50%	4.581%
13	12.898	1829	1838	1843	rBV3	85548	227626	3.80%	0.811%
14	12.957	1843	1848	1851	rVB	6606367	5984146	100.00%	21.309%
15	13.757	1978	1984	1993	rVB	104838	238924	3.99%	0.851%
16	14.004	2022	2026	2029	rBV	1540287	1311779	21.92%	4.671%
17	14.398	2088	2093	2098	rBV2	155188	238157	3.98%	0.848%
18	14.445	2098	2101	2105	rVV5	63707	88020	1.47%	0.313%
19	14.974	2186	2191	2198	rVB2	111551	194604	3.25%	0.693%
20	15.127	2214	2217	2225	rVB2	54032	67051	1.12%	0.239%
21	15.468	2270	2275	2279	rBV	896500	1088541	18.19%	3.876%
22	15.504	2279	2281	2286	rVB	58518	72256	1.21%	0.257%
23	15.615	2295	2300	2307	rVB2	93012	190113	3.18%	0.677%
24	15.945	2352	2356	2361	rBV3	55922	77562	1.30%	0.276%
25	16.368	2422	2428	2435	rVB3	61613	125212	2.09%	0.446%

Sum of corrected areas: 28082816

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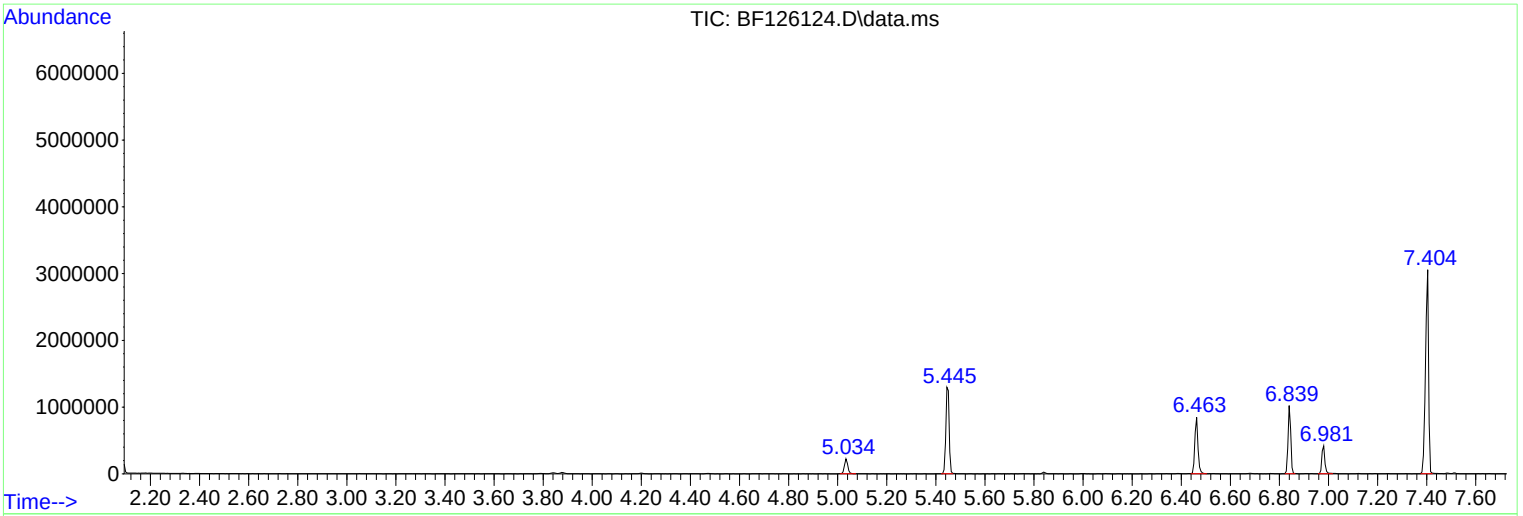
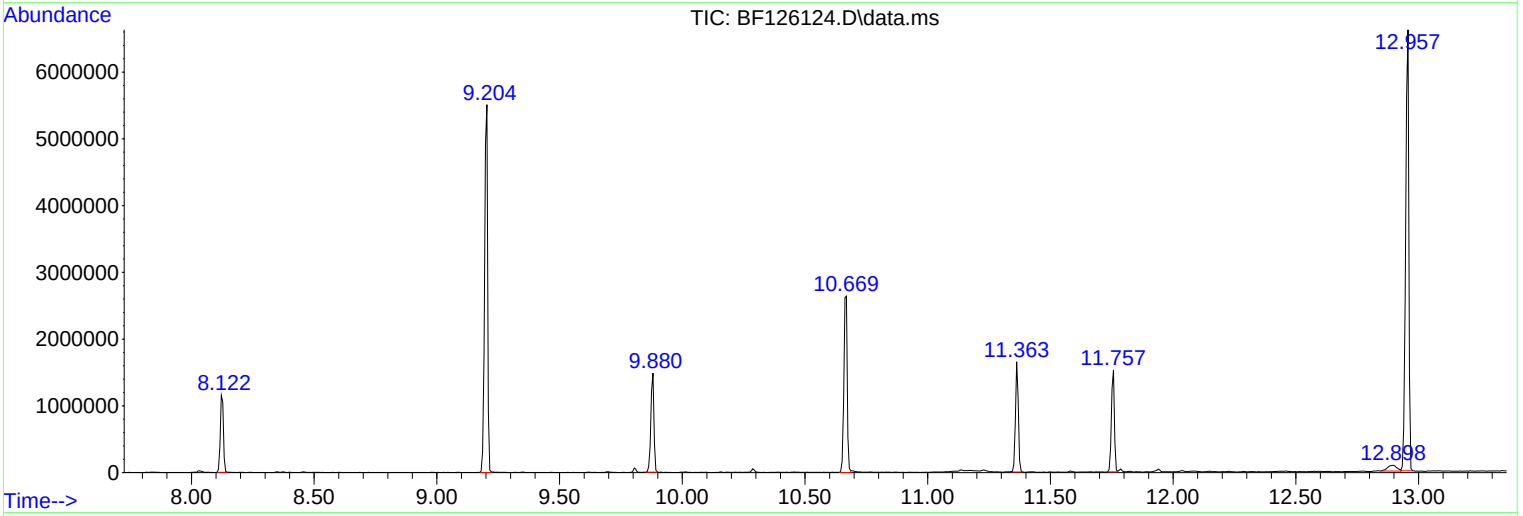
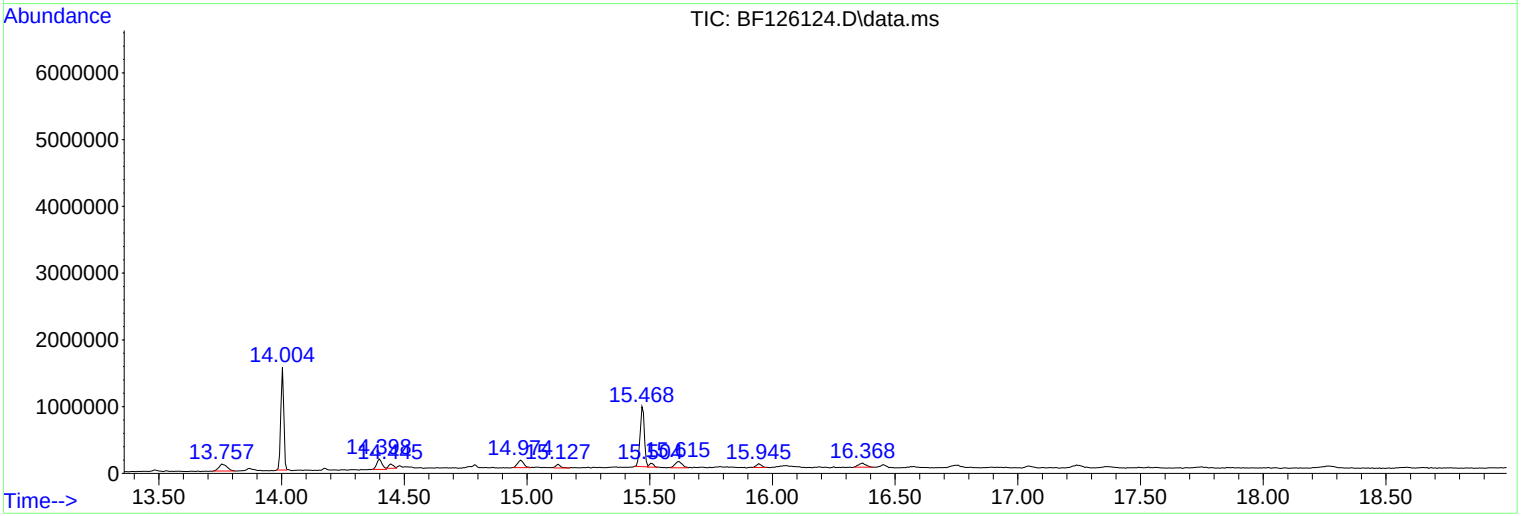
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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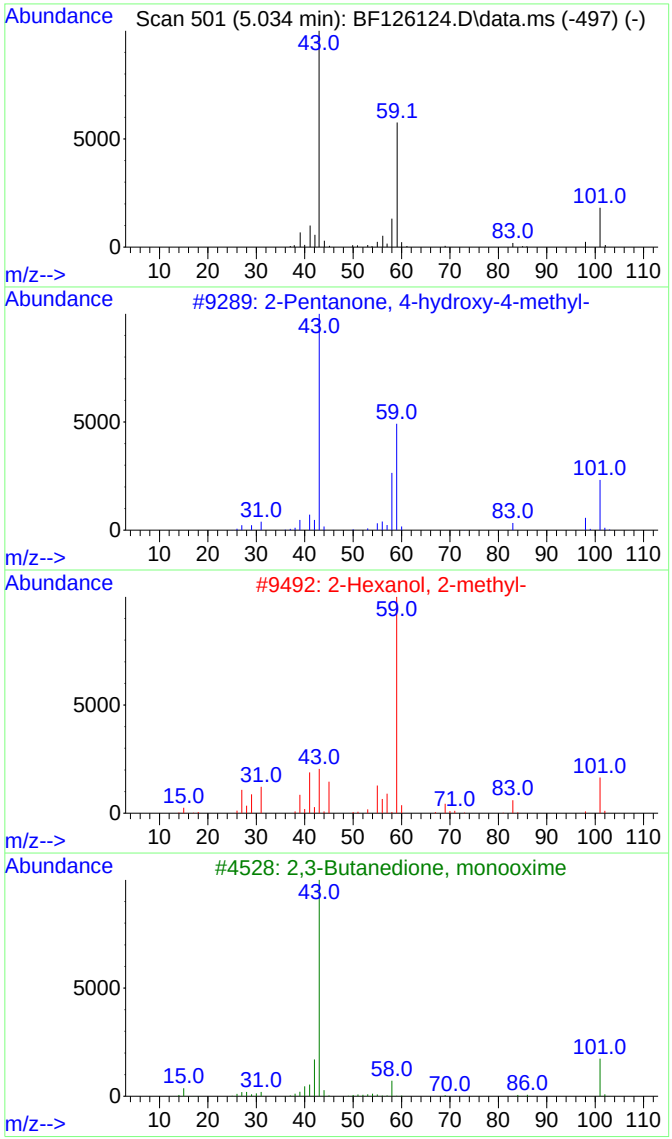
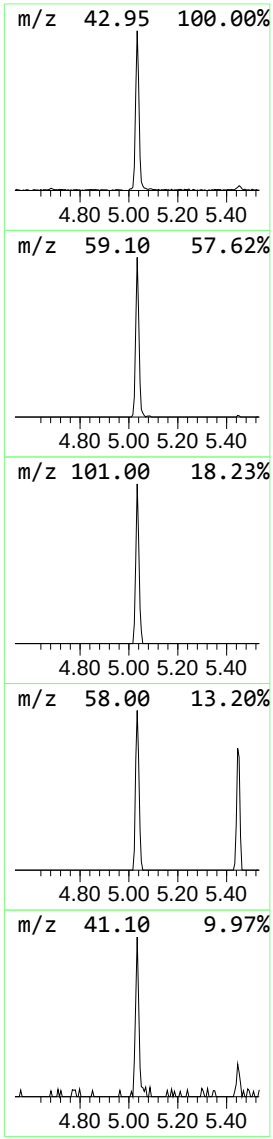
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	5.49 ng	215394	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2-Pentanone	86	C5H10O	000107-87-9	10





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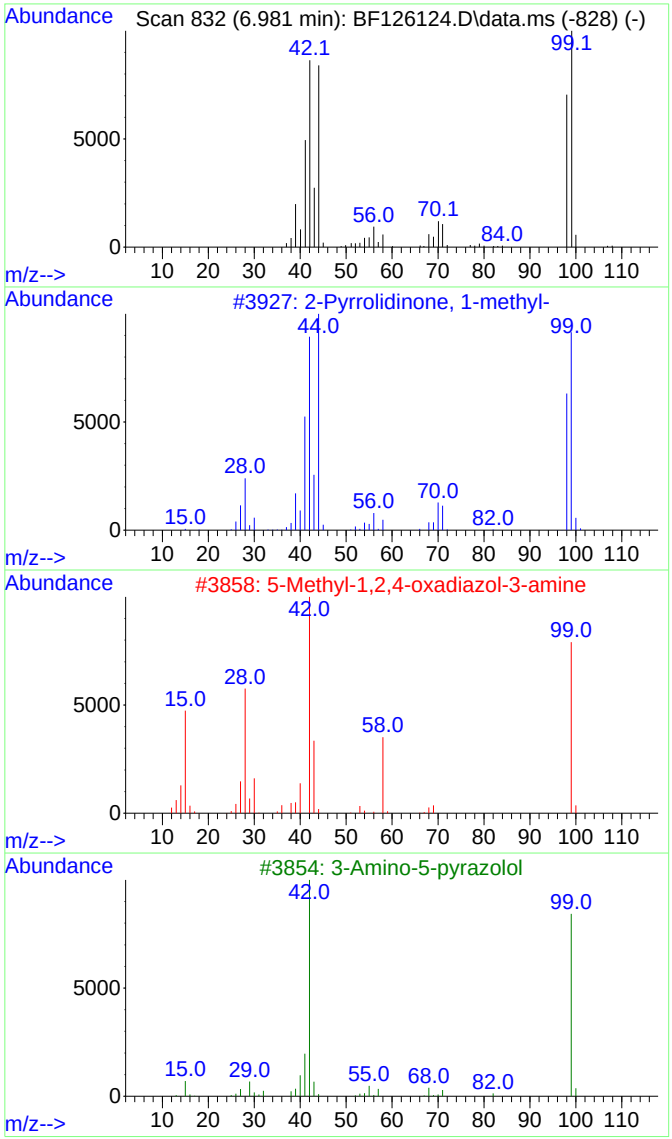
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

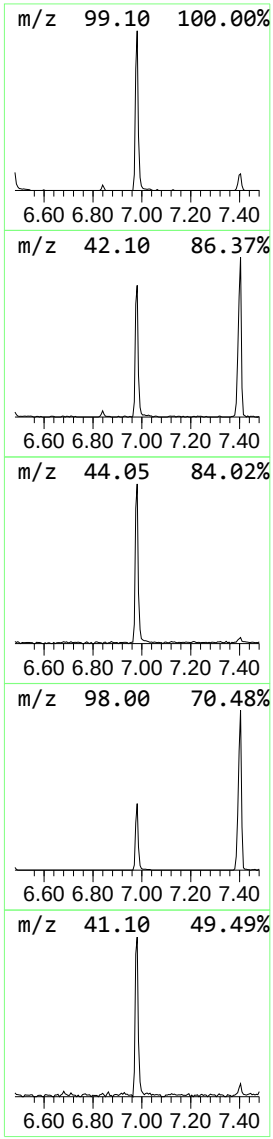
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	9.16 ng	359044	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	97
2	5-Methyl-1,2,4-oxadiazol-3-amine	99	C3H5N3O	040483-47-4	38
3	3-Amino-5-pyrazolol	99	C3H5N3O	006126-22-3	38
4	4H-1,2,4-Triazol-3-amine, 4-methyl-	98	C3H6N4	016681-76-8	27
5	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	25





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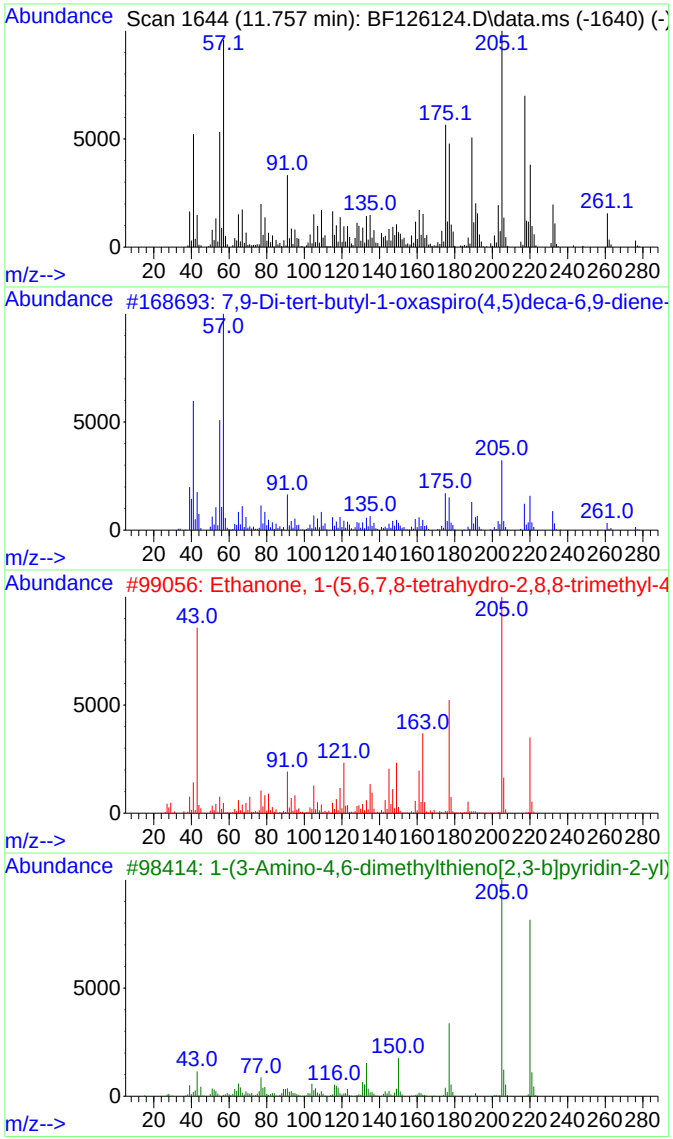
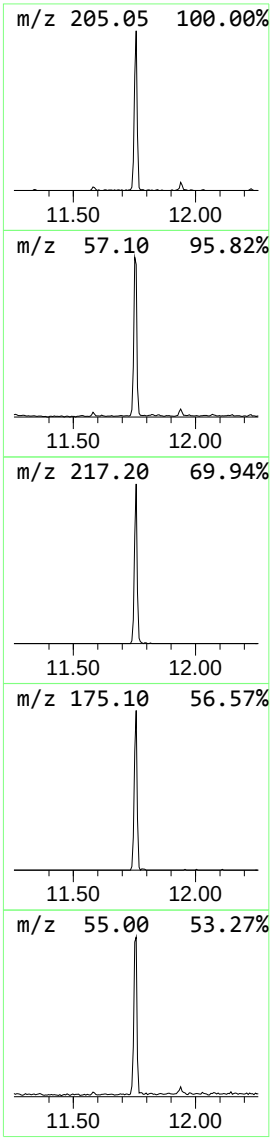
****
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.757	19.35 ng	1286500	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
4	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	45
5	Benzenethanol, O,.beta.,.beta.,2...	220	C15H24O	1010128-94-8	45





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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
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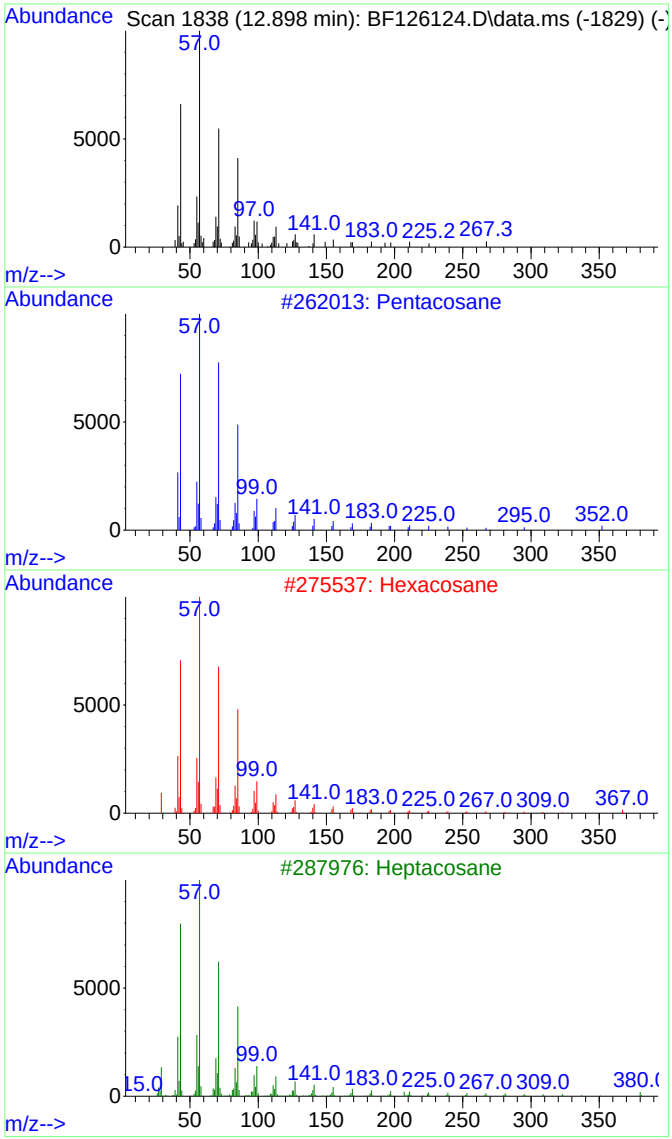
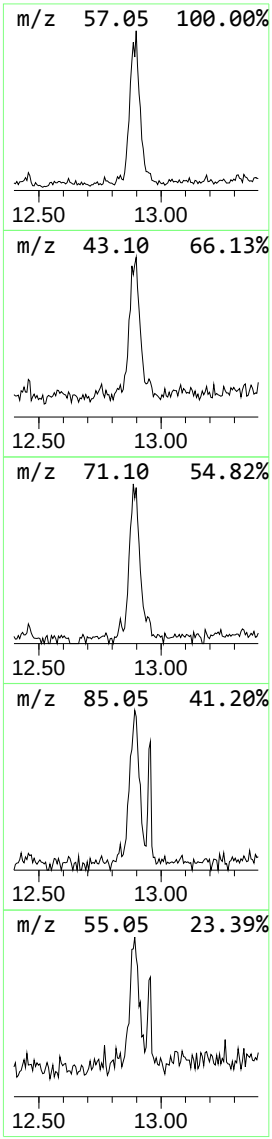
****

Peak Number 4 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.898	3.47 ng	227626	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Sample : M4576-06
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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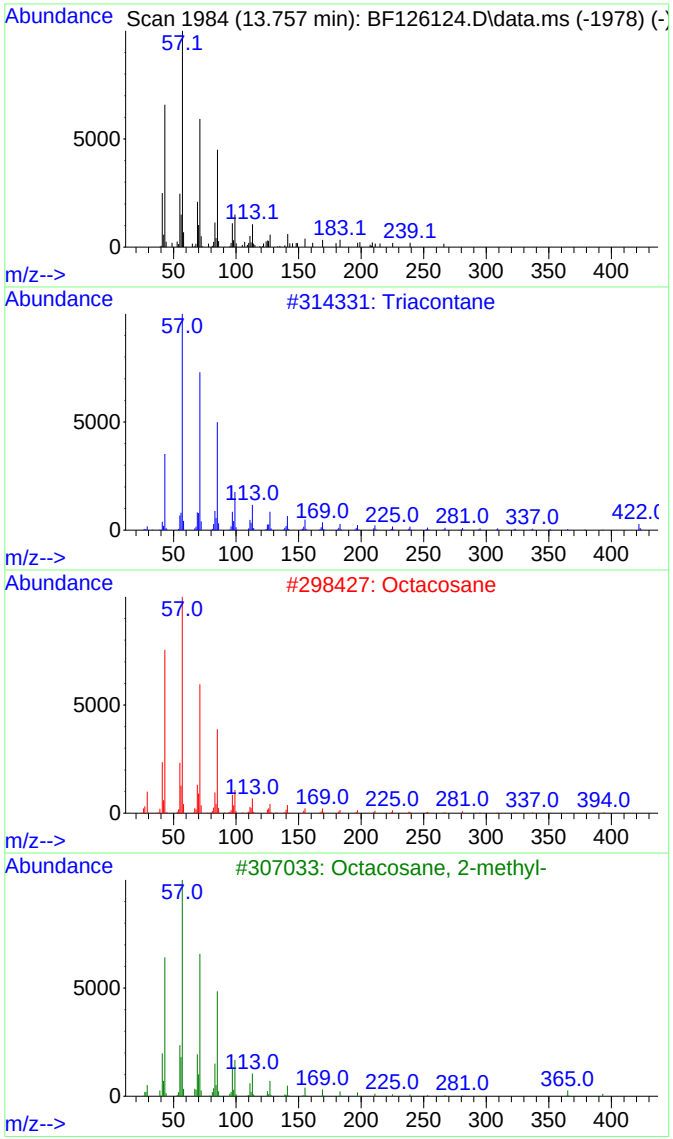
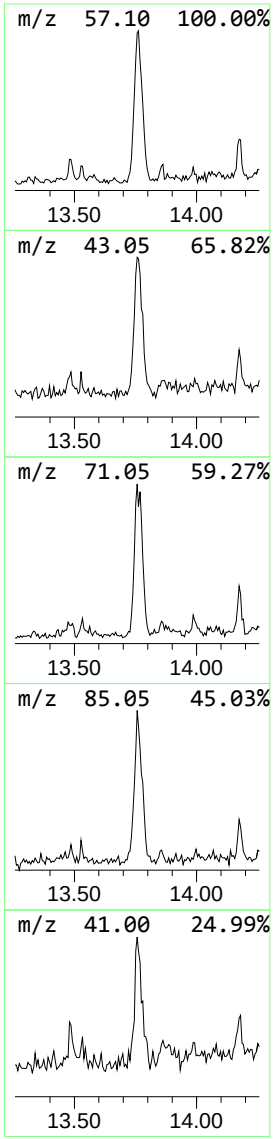
Peak Number 5 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	3.64 ng	238924	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hentriacontane	437	C31H64	000630-04-6	91





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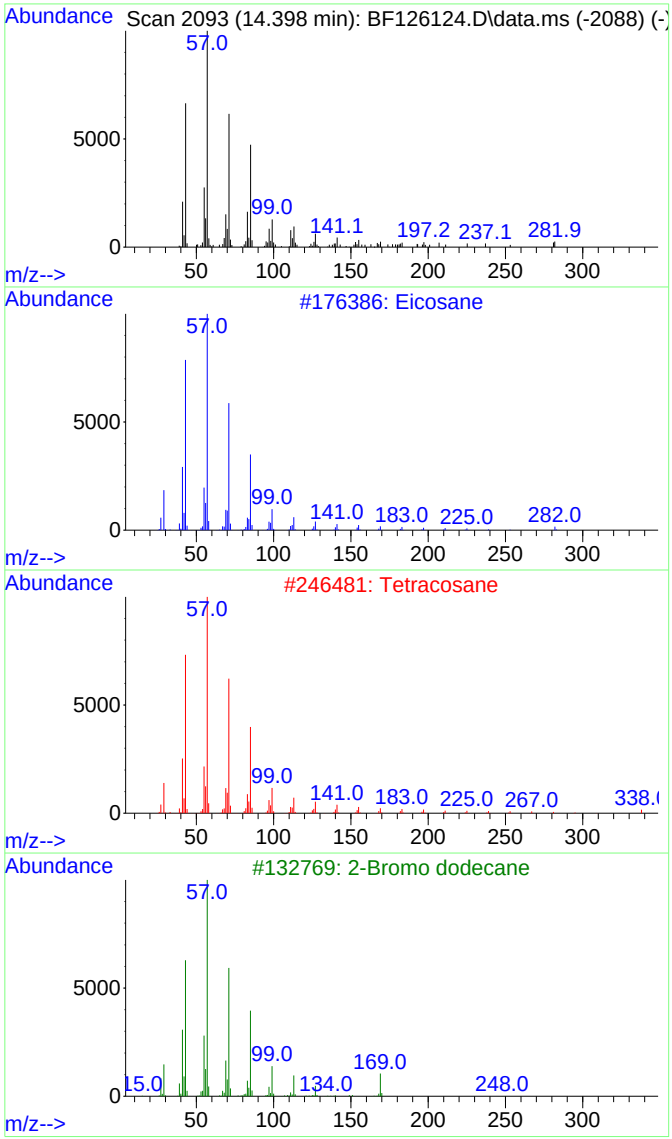
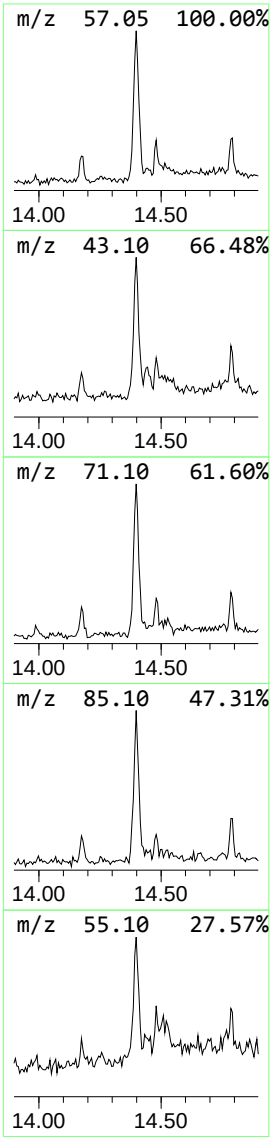
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	3.63 ng	238157	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tetracosane	338	C24H50	000646-31-1	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	87





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

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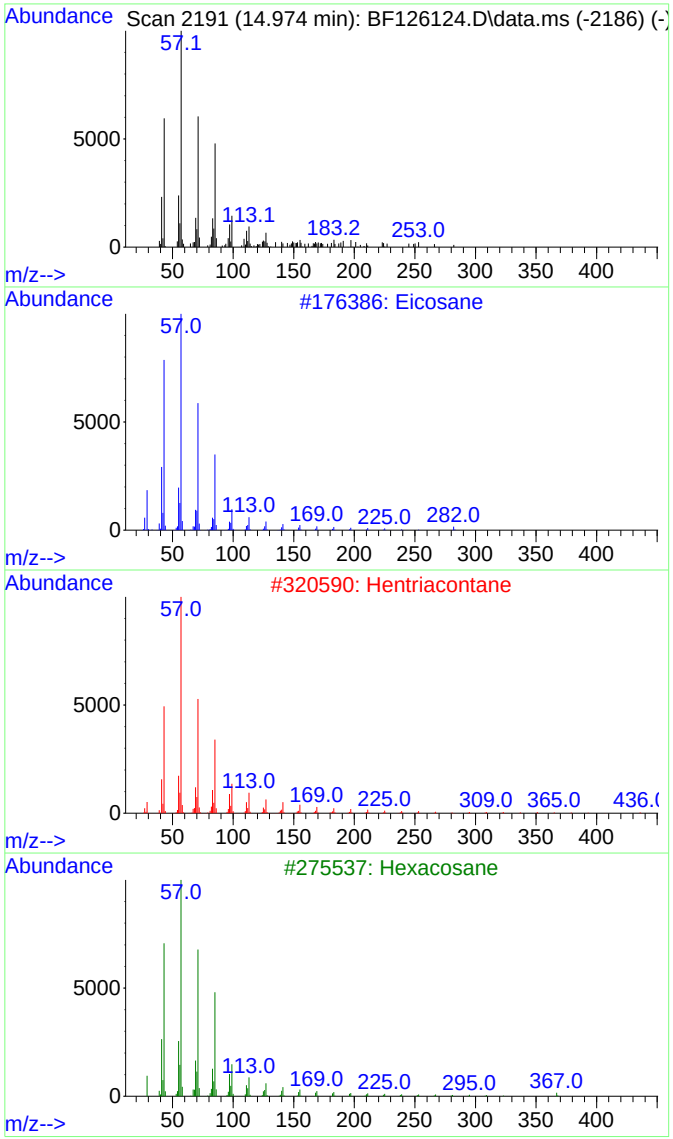
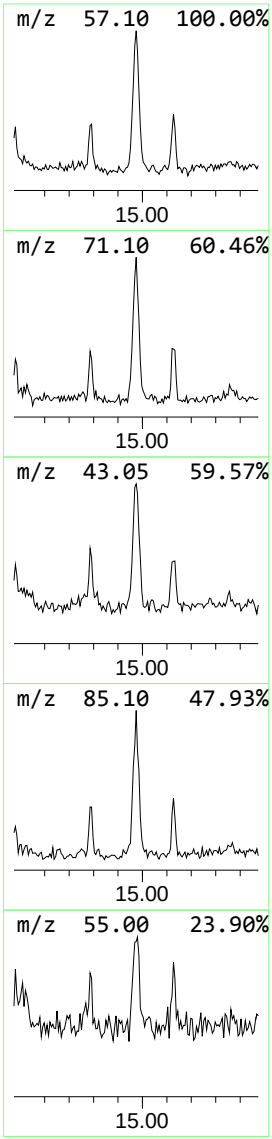
Peak Number 7 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	3.58 ng	194604	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetracosane	338	C24H50	000646-31-1	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





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TIC Library : C:\Database\NIST20.L
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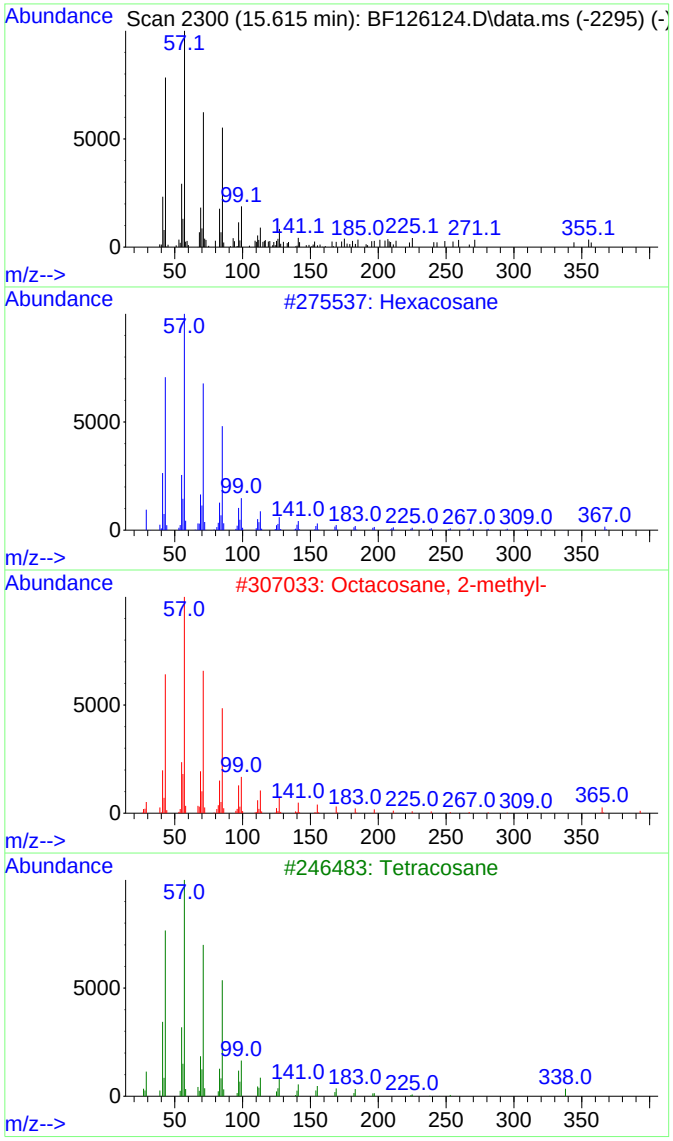
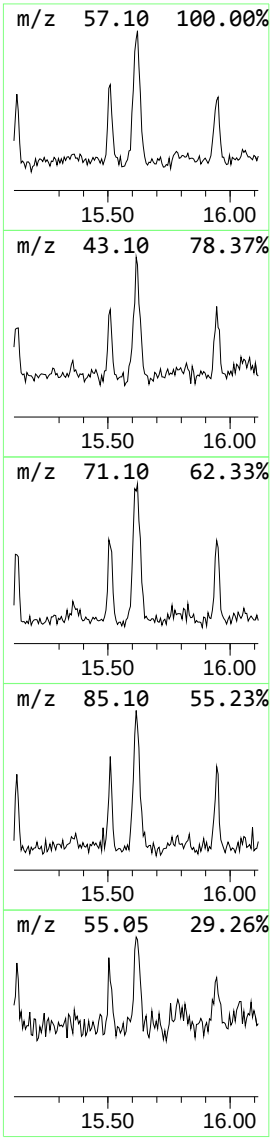
Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	3.49 ng	190113	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Pentacosane	352	C25H52	000629-99-2	86





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Instrument :
BNA_F
ClientSampleId :
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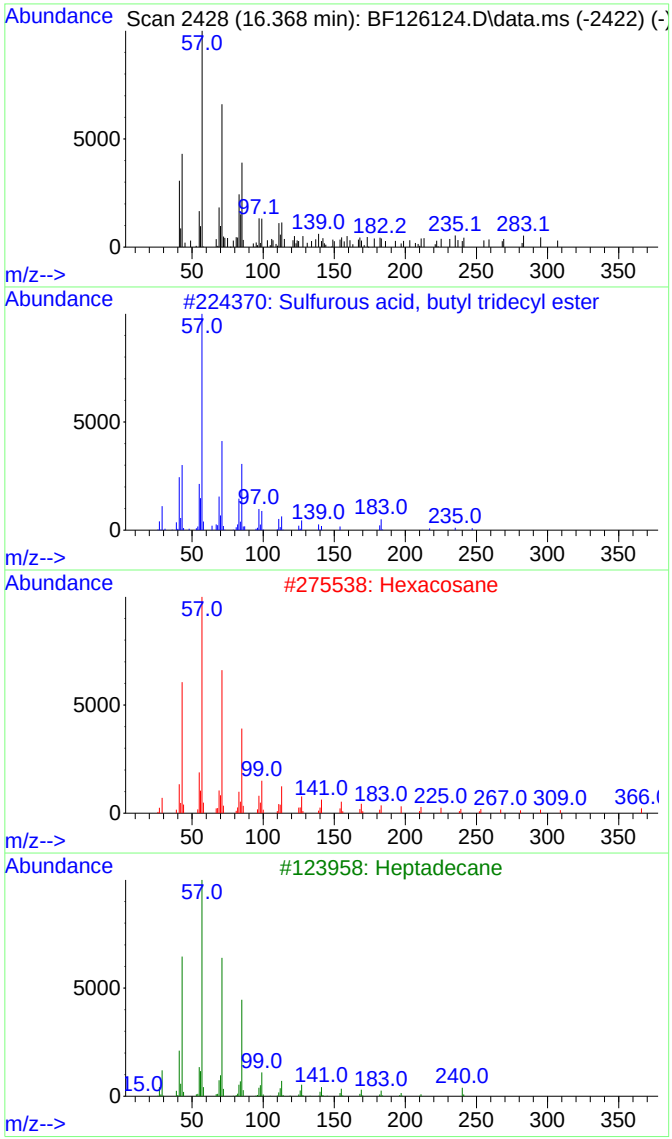
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

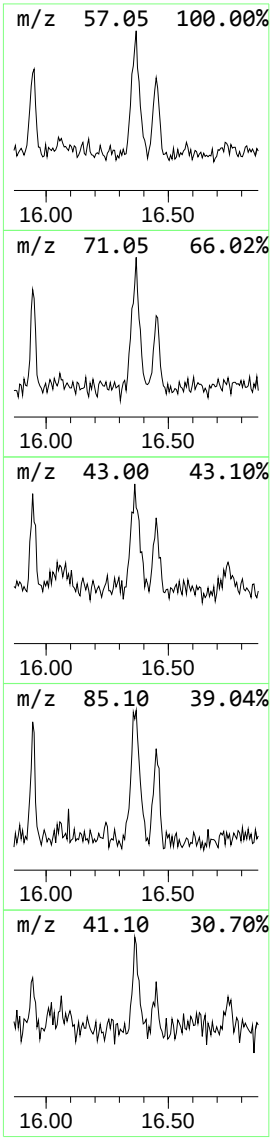
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, butyl tride... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.368	2.30 ng	125212	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	86
2	Hexacosane	366	C26H54	000630-01-3	72
3	Heptadecane	240	C17H36	000629-78-7	64
4	Nonadecane	268	C19H40	000629-92-5	64
5	Eicosane	282	C20H42	000112-95-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111121\
Data File : BF126124.D
Acq On : 11 Nov 2021 13:45
Operator : JU/CG
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Misc :
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BNA_F
ClientSampleId :
TW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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-...	5.034	5.5	ng	215394	1	6.839	784307	20.0
2-Pyrrolidinone...	6.981	9.2	ng	359044	1	6.839	784307	20.0
7,9-Di-tert-but...	11.757	19.4	ng	1286500	4	11.363	1329460	20.0
Pentacosane	12.898	3.5	ng	227626	5	14.004	1311780	20.0
Triacontane	13.757	3.6	ng	238924	5	14.004	1311780	20.0
Eicosane	14.398	3.6	ng	238157	5	14.004	1311780	20.0
Hentriacontane	14.974	3.6	ng	194604	6	15.468	1088540	20.0
Hexacosane	15.615	3.5	ng	190113	6	15.468	1088540	20.0
Sulfurous acid,...	16.368	2.3	ng	125212	6	15.468	1088540	20.0