LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041122\
Data File : BF127736.D
Acq On : 11 Apr 2022 14:02
Operator : CG\JU
Sample : N2334-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-18R

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	490	494	501	rVB	81253	90367	1.75%	0.282%
2	5.581	555	560	563	rBV	1983383	1734203	33.61%	5.421%
3	6.575	725	729	732	rBV	1337037	1104100	21.40%	3.451%
4	6.963	791	795	798	rBV	993111	776580	15.05%	2.428%
5	7.528	885	891	894	rBV	2488803	2614990	50.67%	8.175%
6	8.245	1009	1013	1017	rBV	1165894	978929	18.97%	3.060%
7	9.328	1191	1197	1200	rBV	5061001	4667200	90.44%	14.590%
8	10.010	1309	1313	1316	rBV	1319564	1143908	22.17%	3.576%
9	10.798	1443	1447	1451	rBV	2914534	3081831	59.72%	9.634%
10	11.504	1563	1567	1570	rBV	1229106	1142239	22.13%	3.571%
11	12.016	1651	1654	1658	rBV	128737	124447	2.41%	0.389%
12	12.604	1747	1754	1770	rBV	3414556	5160373	100.00%	16.132%
13	12.933	1807	1810	1821	rVB	67100	85943	1.67%	0.269%
14	13.092	1833	1837	1841	rBV	3770769	3862814	74.86%	12.075%
15	13.615	1920	1926	1942	rBV	2544617	3386586	65.63%	10.587%
16	14.004	1989	1992	1999	rVB2	146919	233182	4.52%	0.729%
17	14.151	2014	2017	2021	rVB	873567	735922	14.26%	2.301%
18	14.498	2073	2076	2091	rVB	132437	235408	4.56%	0.736%
19	15.686	2272	2278	2284	rVB	618623	830215	16.09%	2.595%

Sum of corrected areas: 31989237

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Misc :
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Instrument :
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ClientSampleId :
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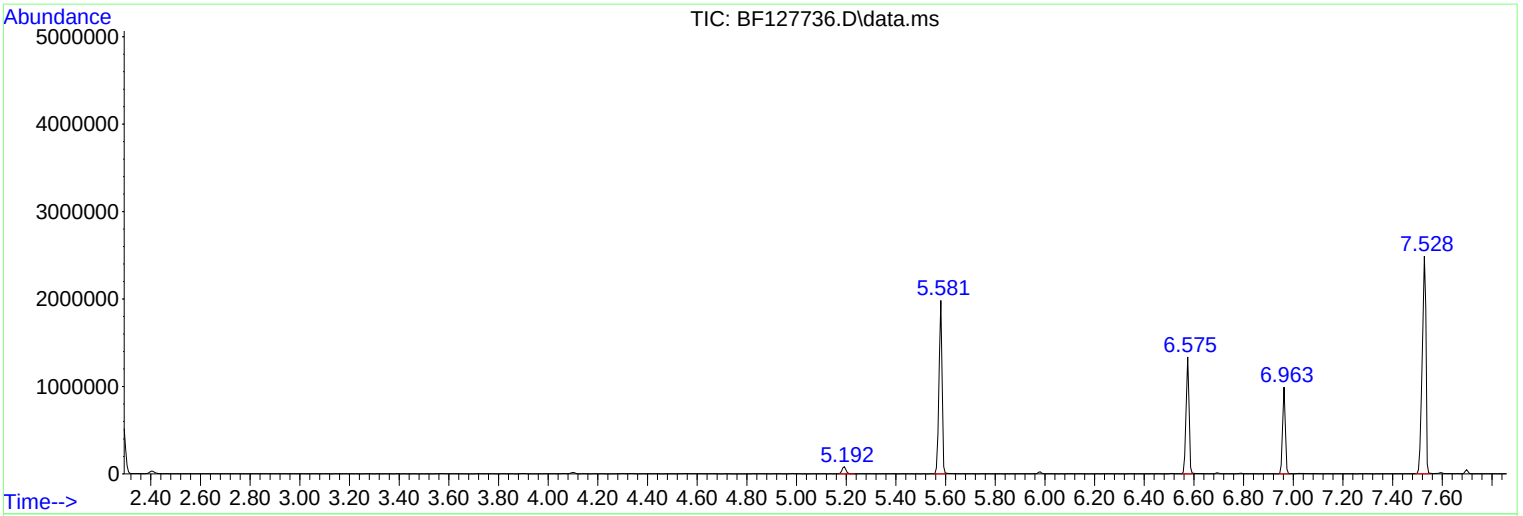
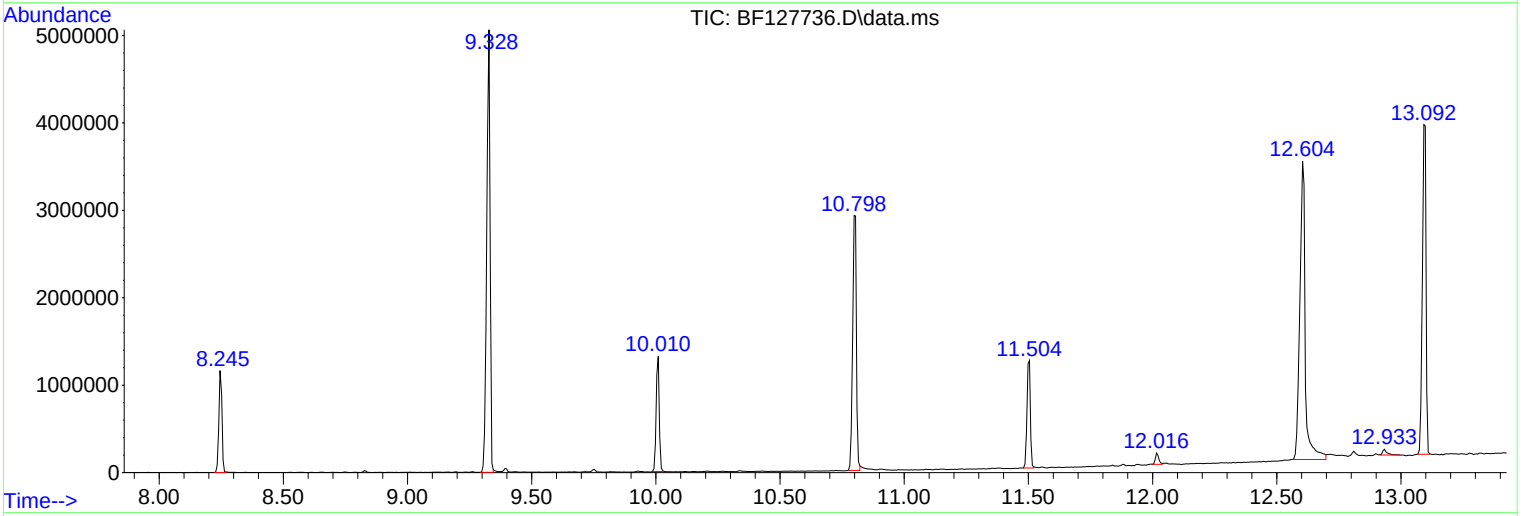
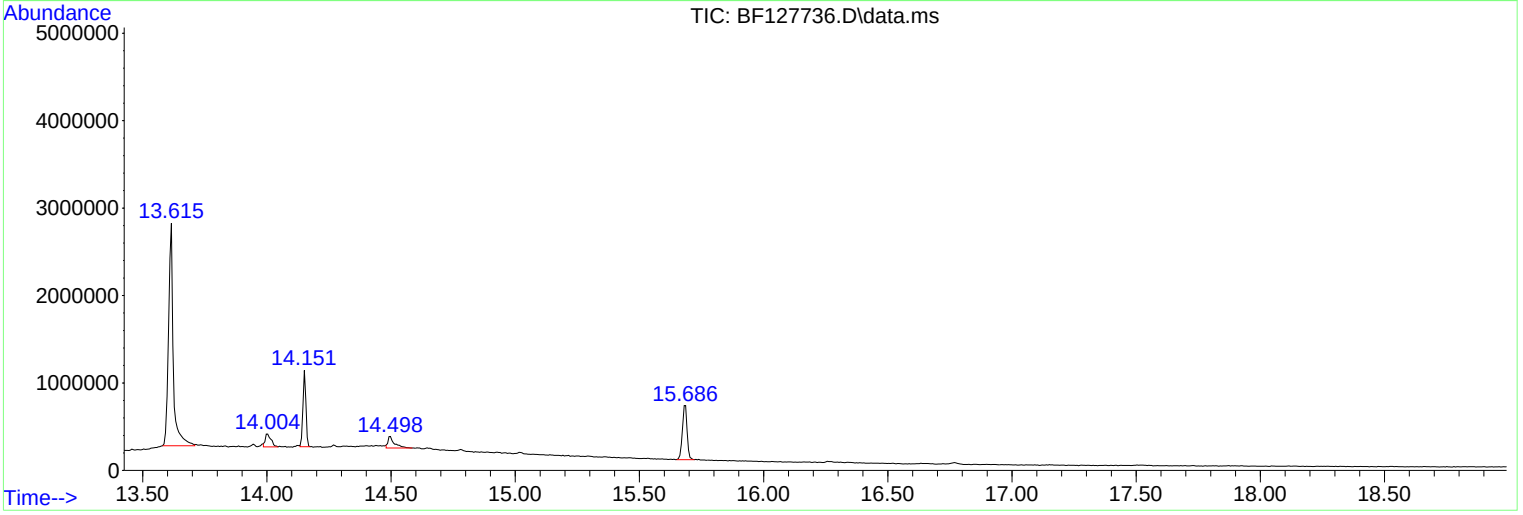
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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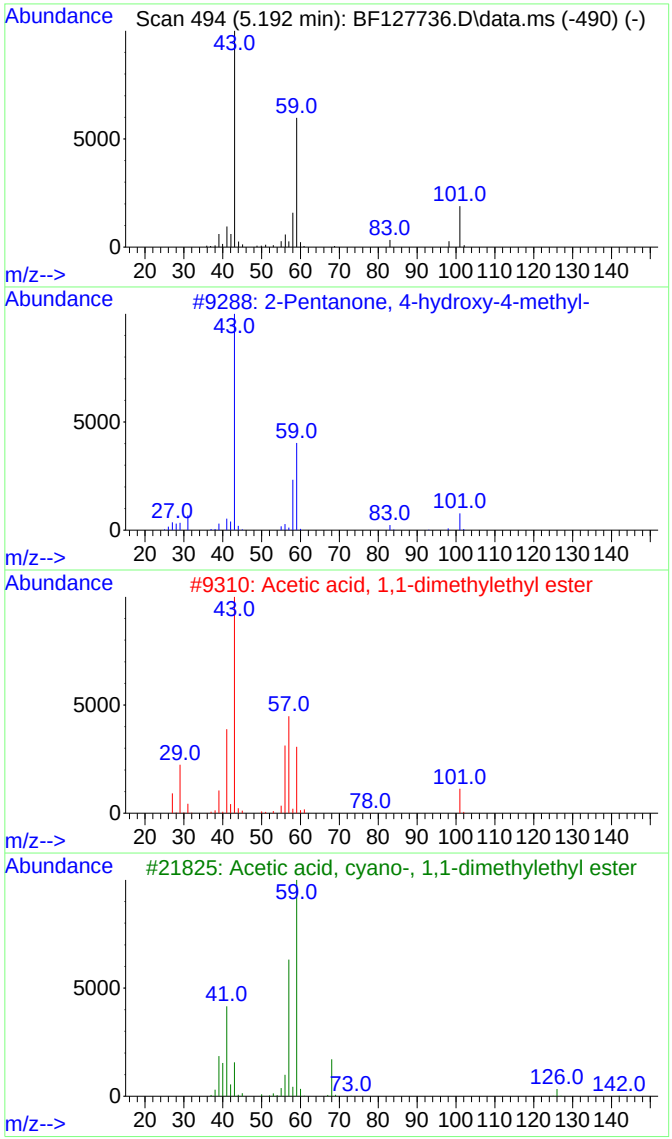
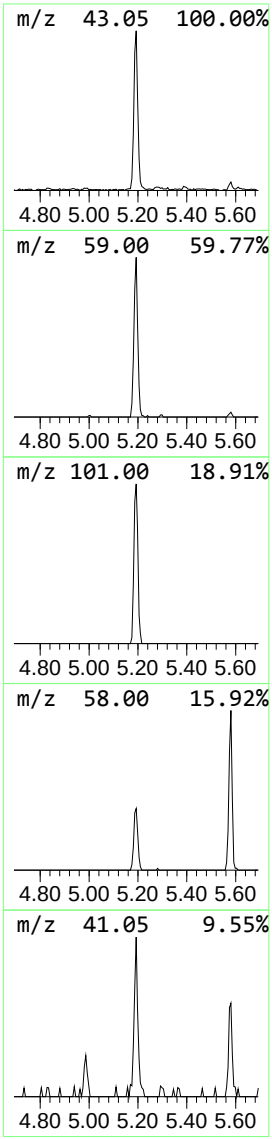
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	2.33 ng	90367	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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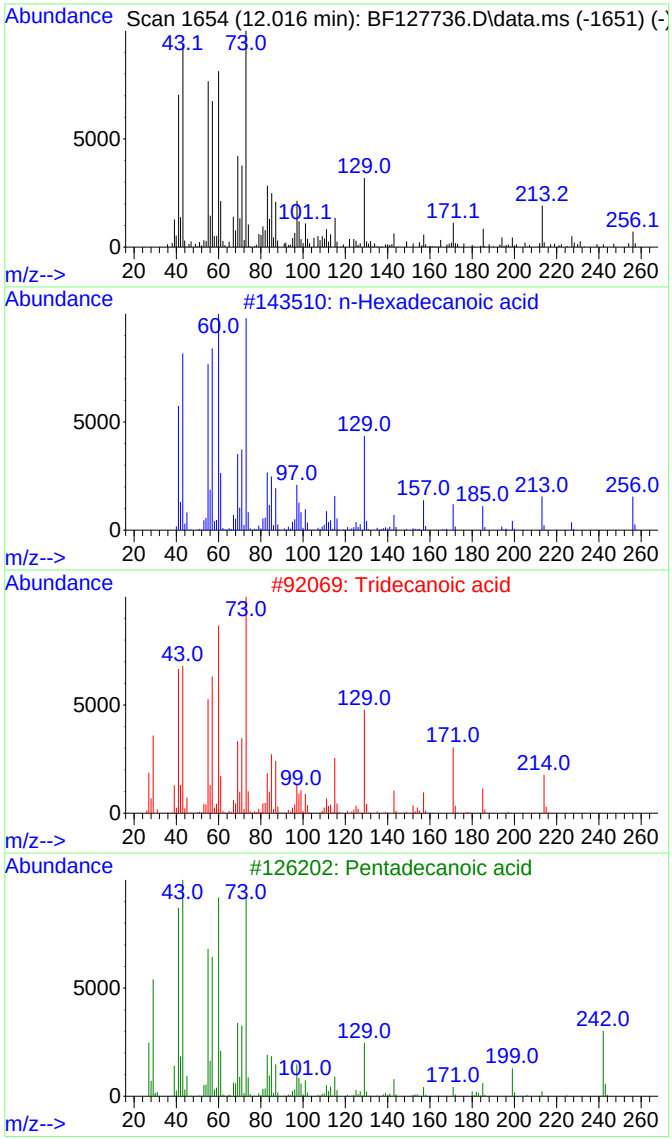
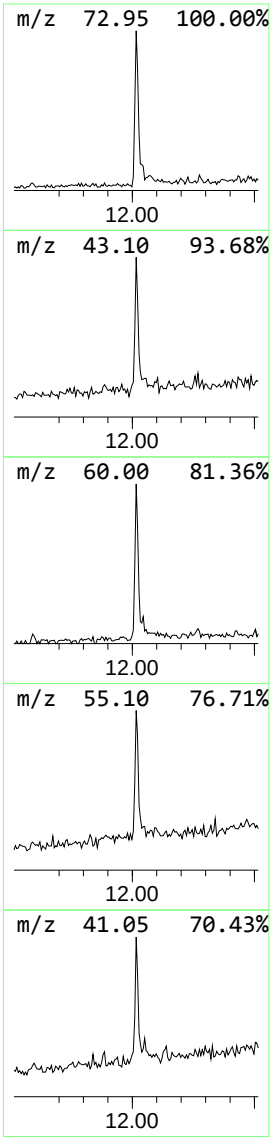
Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	2.18 ng	124447	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Operator : CG\JU
Sample : N2334-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-18R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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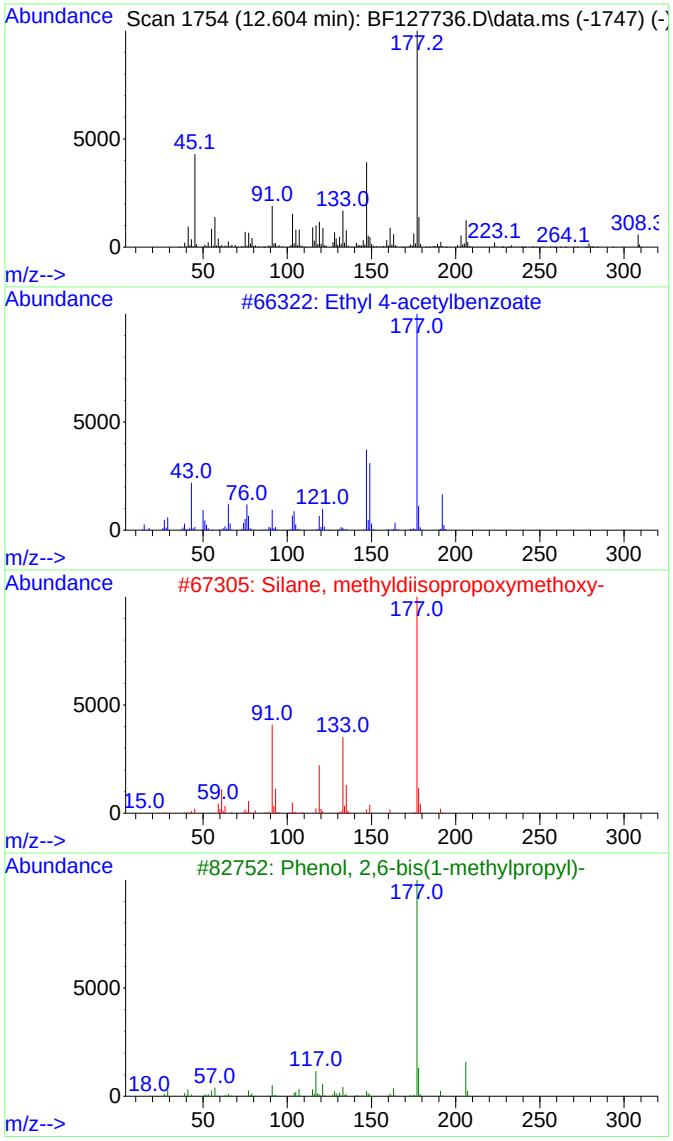
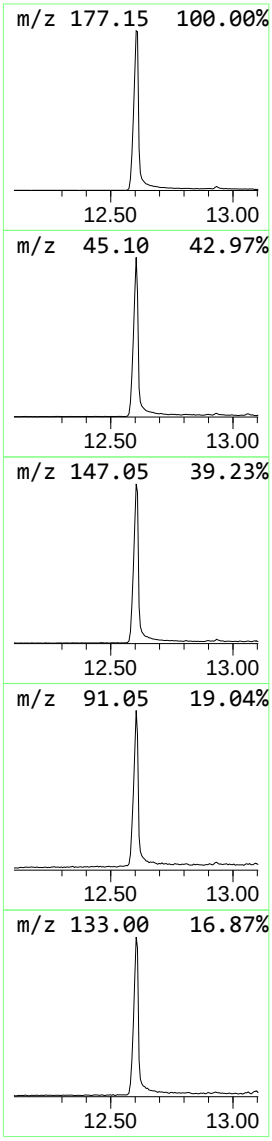
Peak Number 3 Ethyl 4-acetylbenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	90.36 ng	5160370	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 4-acetylbenzoate	192	C11H12O3	038430-55-6	50
2	Silane, methyldiisopropoxymethoxy-	192	C8H20O3Si	1000416-18-5	50
3	Phenol, 2,6-bis(1-methylpropyl)-	206	C14H22O	005510-99-6	45
4	Spiro[cyclopenta[d]-1,3,2-dioxab...	206	C12H19BO2	062238-26-0	41
5	1-Cyclohexanone,3,3-dimethyl-2-[...	236	C15H24O2	1000196-83-5	40





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
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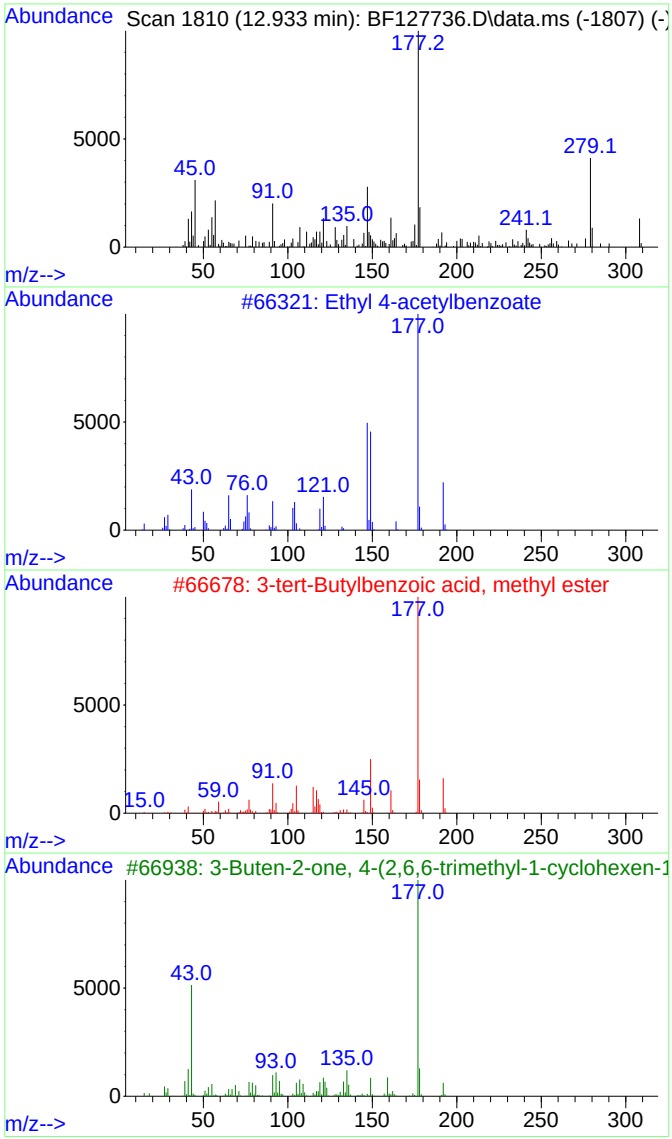
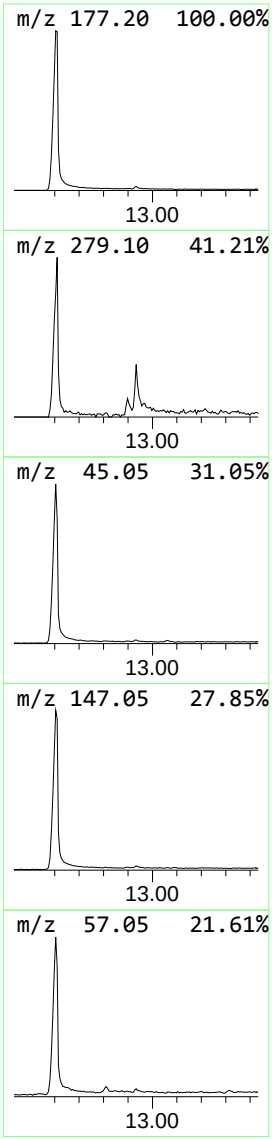
Peak Number 4 unknown12.933 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.933	2.34 ng	85943	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 4-acetylbenzoate	192	C11H12O3	038430-55-6	43
2	3-tert-Butylbenzoic acid, methyl...	192	C12H16O2	027330-57-0	38
3	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	35
4	7-Methoxy-2-methyl-1,2,3,4-tetra...	177	C11H15NO	054893-23-1	35
5	2,6-Diamino-4-cyclohexyl-4H-thio...	260	C13H16N4S	1000293-91-8	35





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Instrument :
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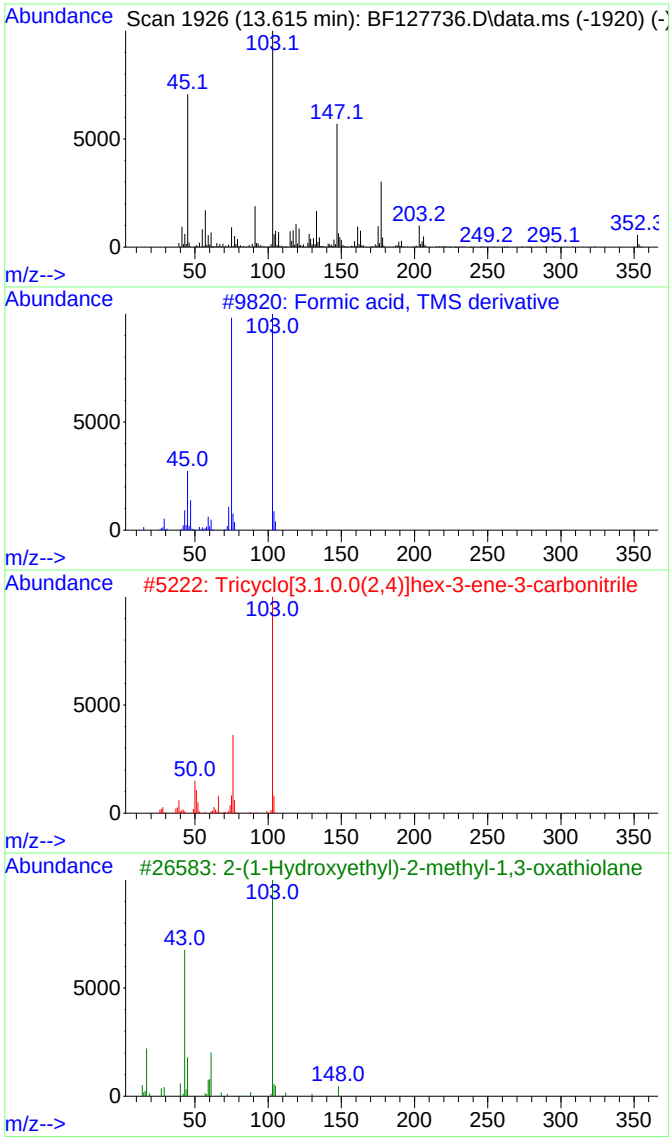
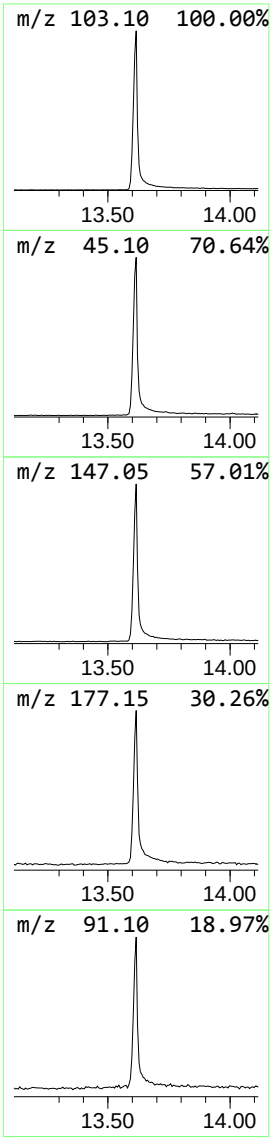
Peak Number 5 unknown13.616 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.616	92.04 ng	3386590	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, TMS derivative	118	C4H10O2Si	018243-21-5	32
2	Tricyclo[3.1.0.0(2,4)]hex-3-ene-...	103	C7H5N	103495-51-8	22
3	2-(1-Hydroxyethyl)-2-methyl-1,3-...	148	C6H12O2S	107903-37-7	16
4	Nootkatone	218	C15H22O	004674-50-4	11
5	1H-Inden-1-ol, 2,3-dihydro-3,3-d...	162	C11H14O	038393-92-9	10





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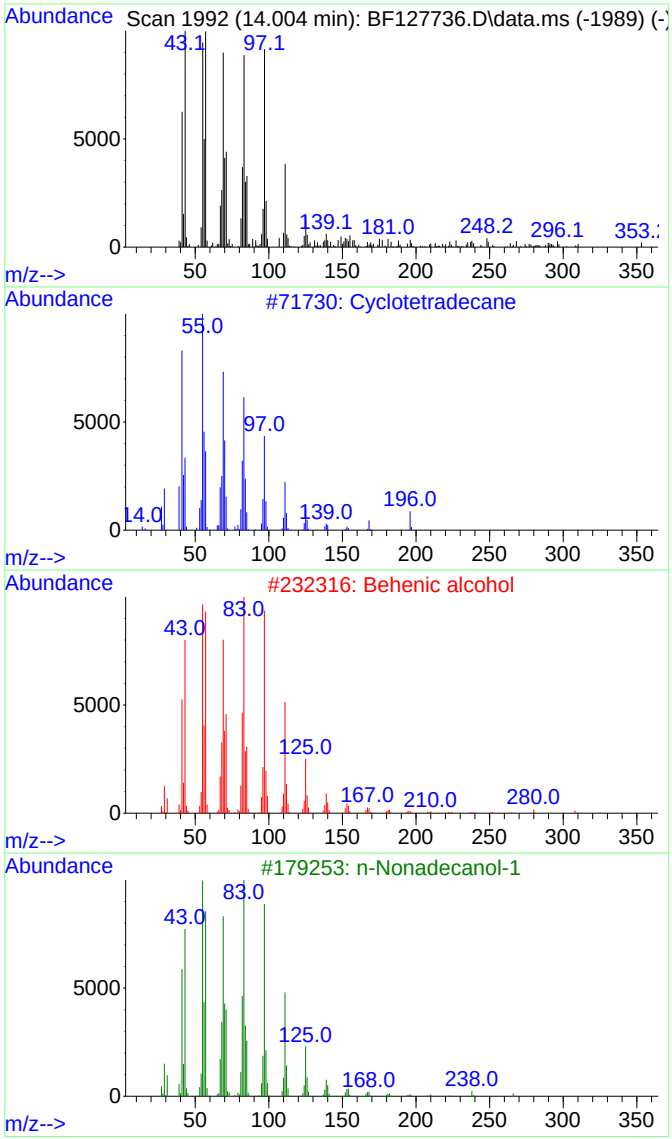
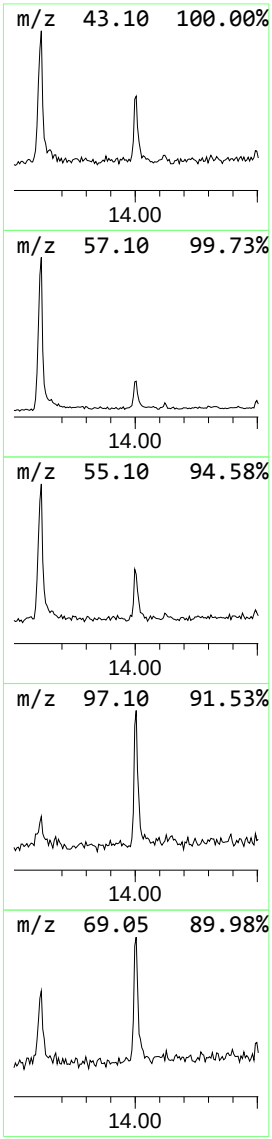
Peak Number 6 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	6.34 ng	233182	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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TIC Library : C:\Database\NIST20.L
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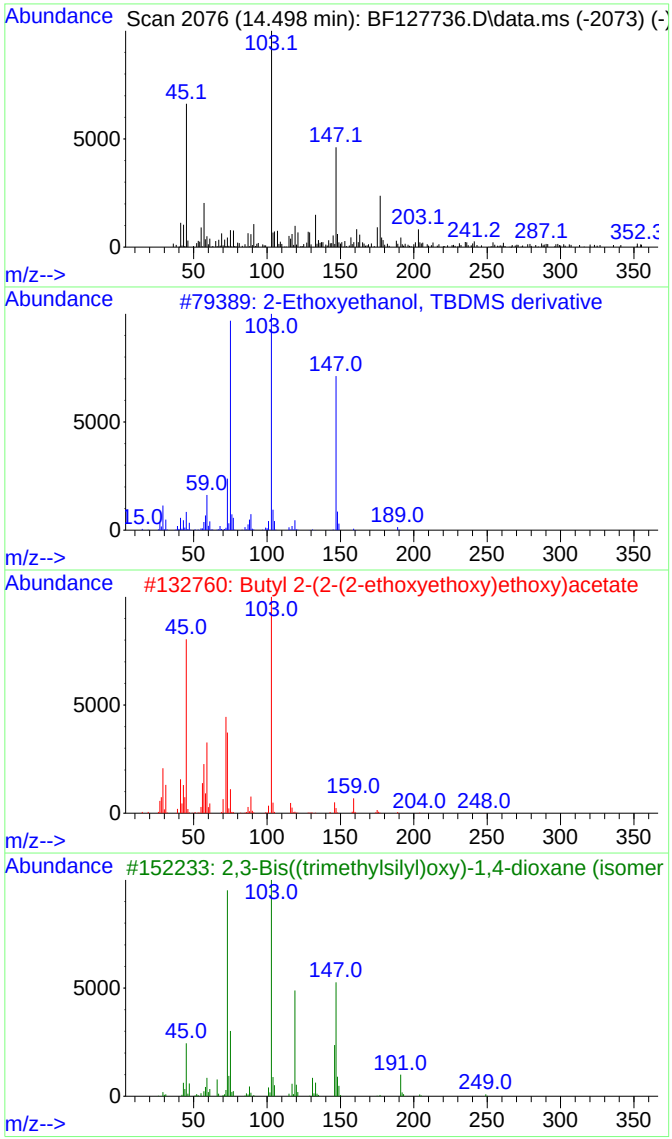
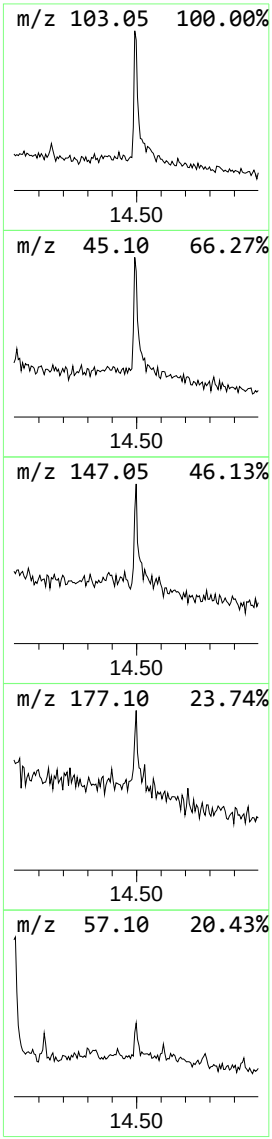
Peak Number 7 unknown14.498 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	6.40 ng	235408	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethoxyethanol, TBDMS derivative	204	C10H24O2Si	1000352-13-6	38
2	Butyl 2-(2-(2-ethoxyethoxy)ethox...	248	C12H24O5	1000366-77-5	38
3	2,3-Bis((trimethylsilyl)oxy)-1,4...	264	C10H24O4Si2	1000473-39-0	28
4	2-(1-Hydroxyethyl)-2-methyl-1,3-...	148	C6H12O2S	107903-37-7	27
5	Dibutyl 3,6,9,12-tetraoxatetrade...	378	C18H34O8	1010366-80-2	25





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.192	2.3	ng	90367	1	6.963	776580	20.0
n-Hexadecanoic ...	12.016	2.2	ng	124447	4	11.504	1142240	20.0
Ethyl 4-acetylb...	12.604	90.4	ng	5160370	4	11.504	1142240	20.0
unknown12.933	12.933	2.3	ng	85943	5	14.151	735922	20.0
unknown13.616	13.616	92.0	ng	3386590	5	14.151	735922	20.0
Cyclotetradecane	14.004	6.3	ng	233182	5	14.151	735922	20.0
unknown14.498	14.498	6.4	ng	235408	5	14.151	735922	20.0