LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128544.D
Acq On : 28 May 2022 13:03
Operator : CG\JU
Sample : N2931-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P009-SS003-2430-01

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	461	472	479	rBV	181823	240787	4.84%	0.687%
2	5.451	533	538	542	rBV	3450670	3773816	75.92%	10.767%
3	6.463	704	710	713	rBV	3646352	3968212	79.83%	11.322%
4	6.839	770	774	777	rBV	1305054	1167104	23.48%	3.330%
5	7.398	864	869	872	rBV	2838953	2809274	56.52%	8.015%
6	8.116	987	991	995	rBV	1667553	1565759	31.50%	4.467%
7	9.198	1169	1175	1178	rBV	5228419	4970671	100.00%	14.182%
8	9.822	1275	1281	1285	rBV	854863	707918	14.24%	2.020%
9	9.875	1285	1290	1293	rBV	2170979	1793716	36.09%	5.118%
10	10.663	1419	1424	1427	rBV	3095746	2788095	56.09%	7.955%
11	10.745	1433	1438	1439	rBV	43181	54240	1.09%	0.155%
12	10.775	1439	1443	1446	rVB	840400	694272	13.97%	1.981%
13	11.363	1539	1543	1546	rBV	2217192	1851576	37.25%	5.283%
14	11.757	1607	1610	1613	rVB	76265	62470	1.26%	0.178%
15	11.886	1629	1632	1637	rBV	94537	100368	2.02%	0.286%
16	12.957	1809	1814	1817	rBV	4719472	4796123	96.49%	13.684%
17	13.892	1968	1973	1987	rVB3	131363	372392	7.49%	1.062%
18	13.998	1987	1991	1995	rBV	1381351	1348331	27.13%	3.847%
19	14.098	2003	2008	2016	rBV	473322	485858	9.77%	1.386%
20	14.868	2135	2139	2144	rBV	333191	354668	7.14%	1.012%
21	15.462	2235	2240	2245	rBV	834084	1082602	21.78%	3.089%
22	15.945	2320	2322	2330	rVB5	34158	61047	1.23%	0.174%

Sum of corrected areas: 35049299

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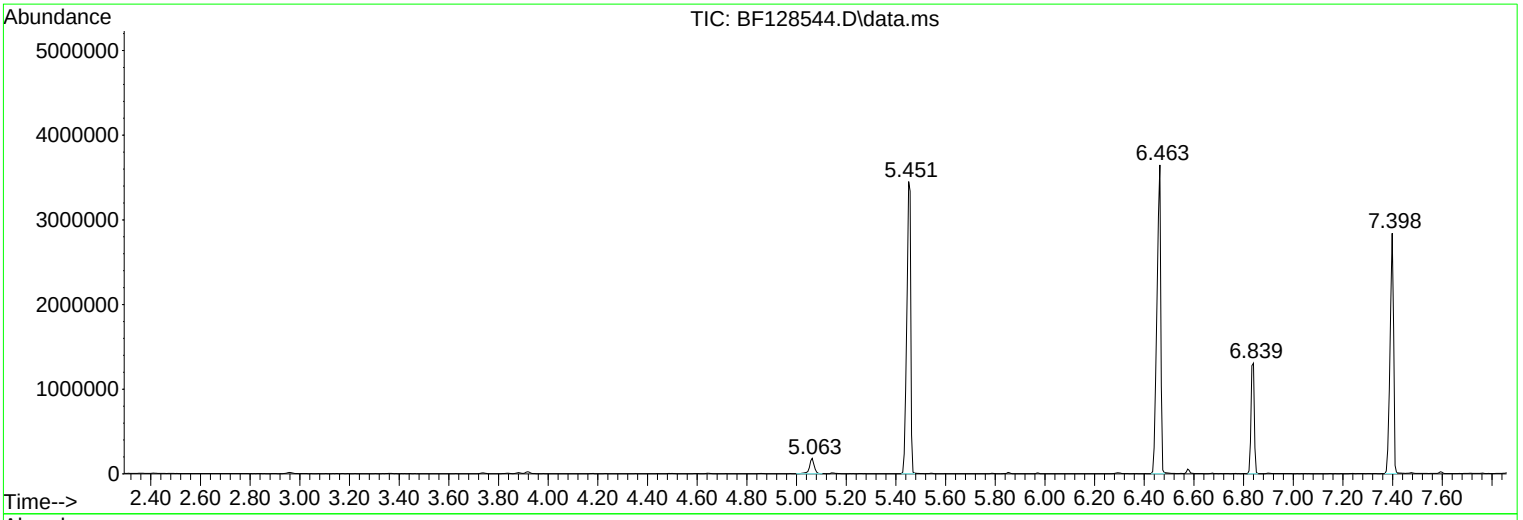
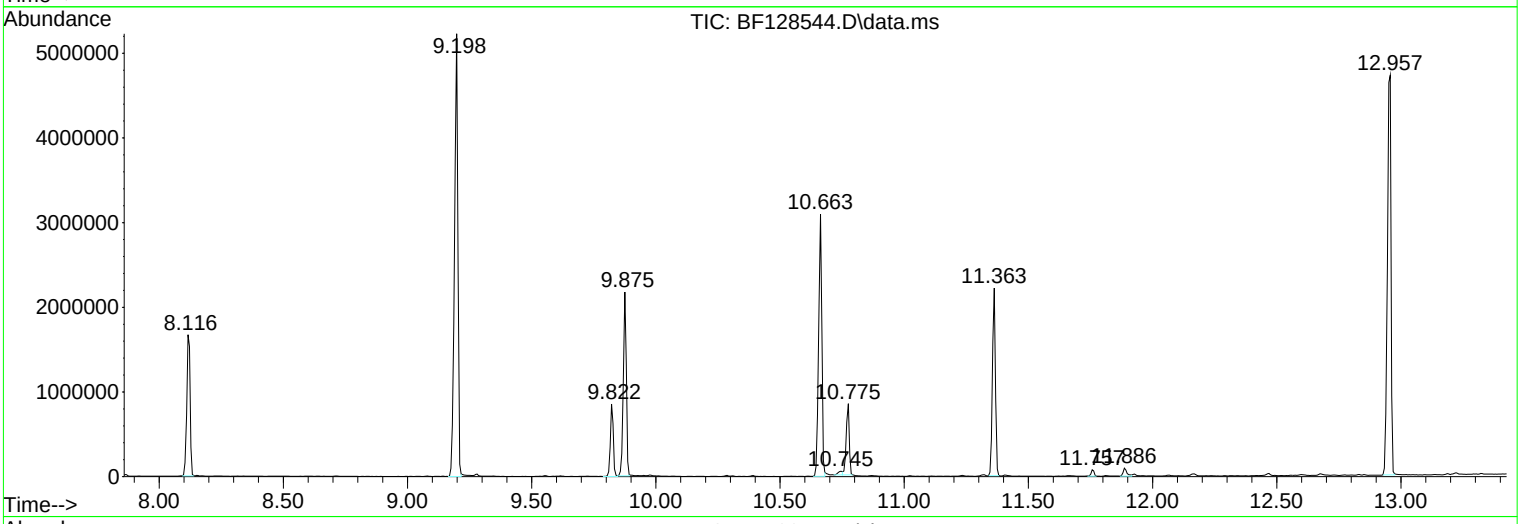
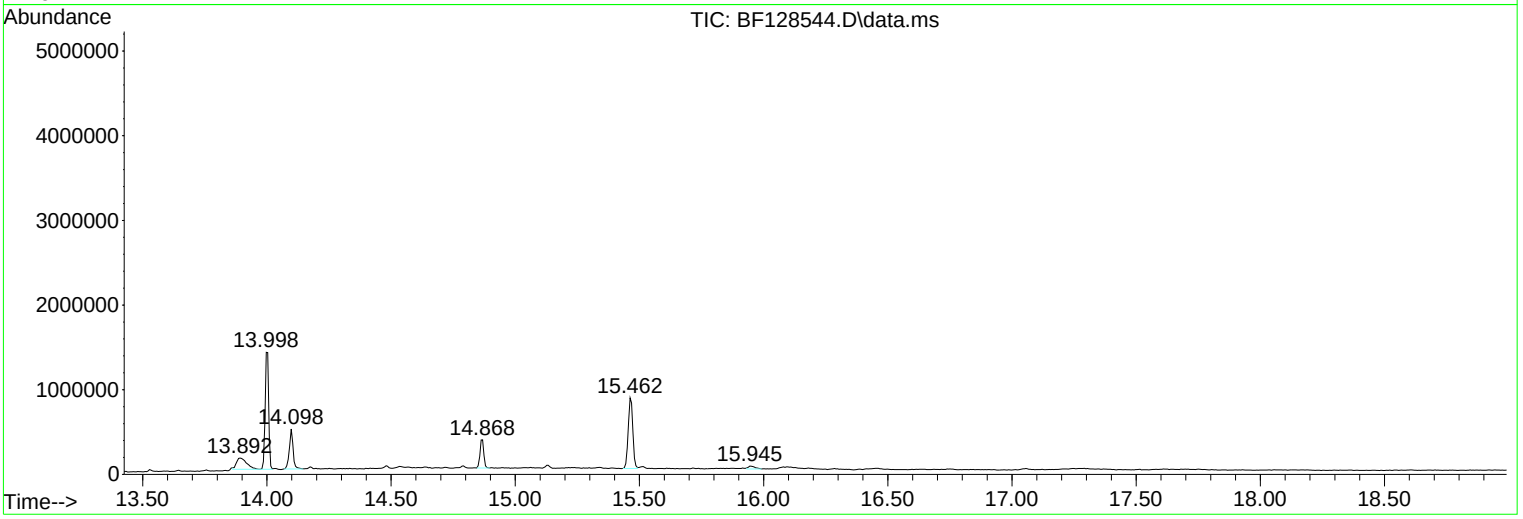
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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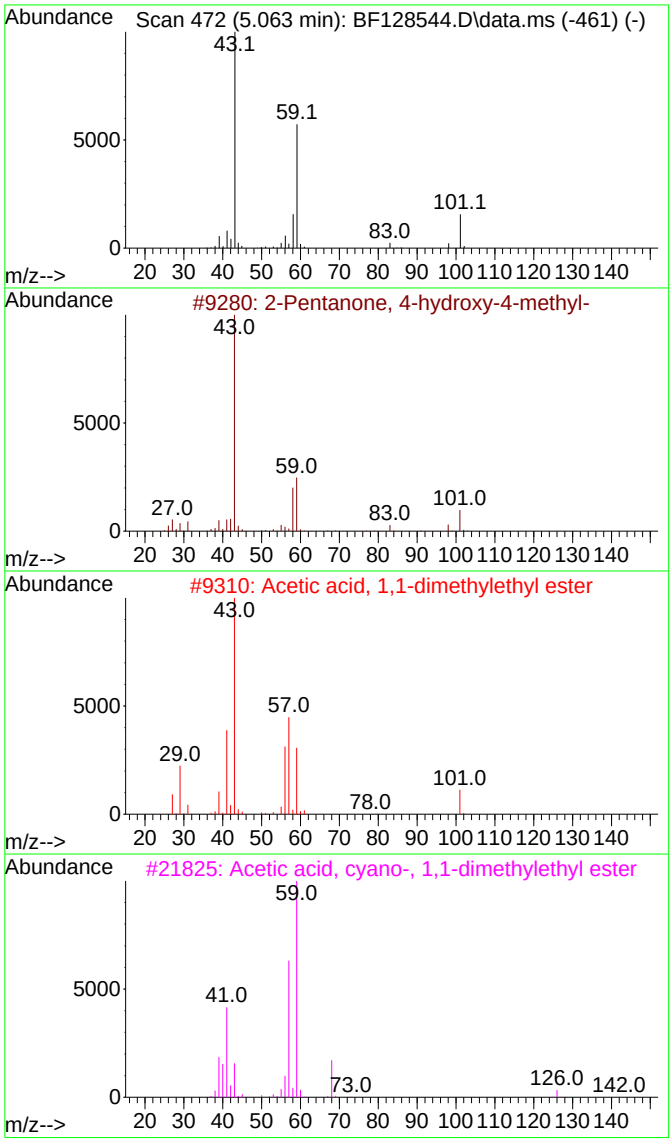
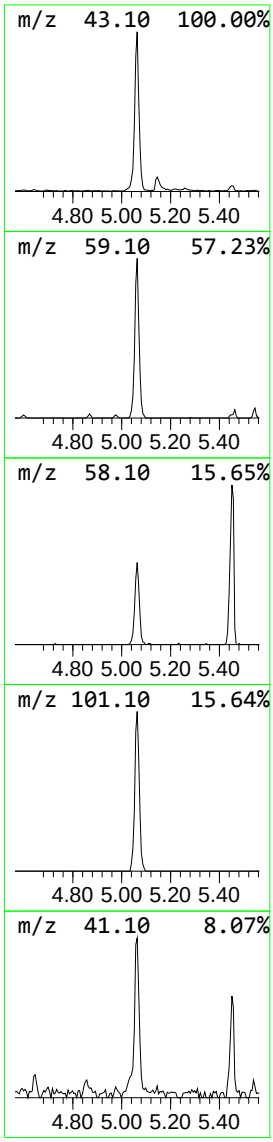
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	4.13 ng	240787	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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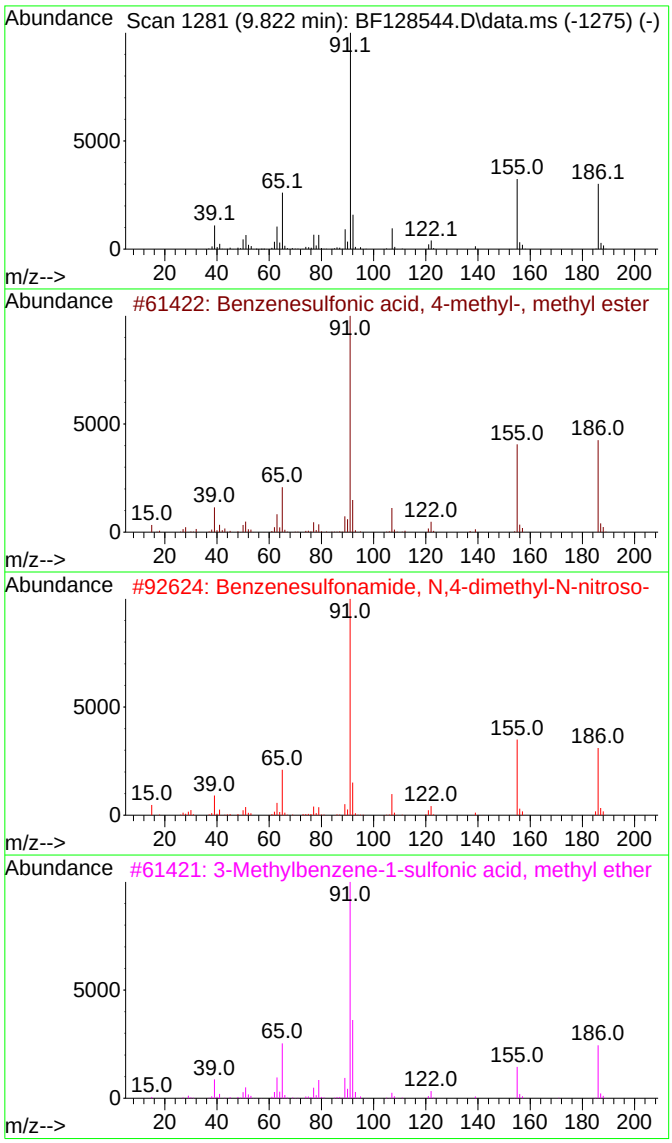
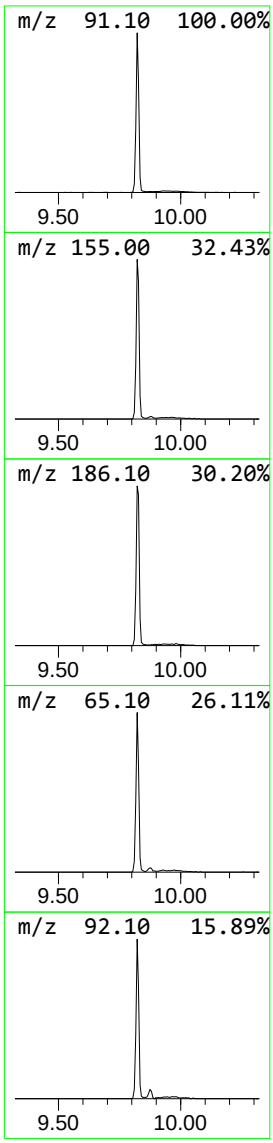
****
Peak Number 2 Benzenesulfonic acid, 4-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.822	7.89 ng	707918	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	94
2	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	91
3	3-Methylbenzene-1-sulfonic acid,...	186	C8H10O3S	126865-07-4	89
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	53
5	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50





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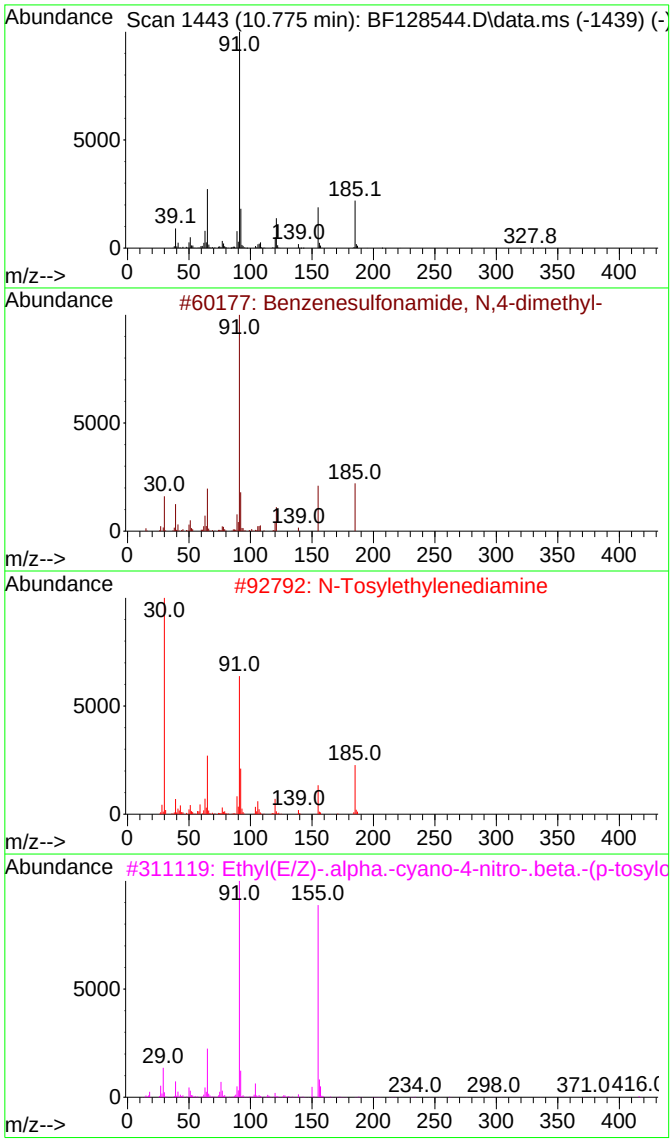
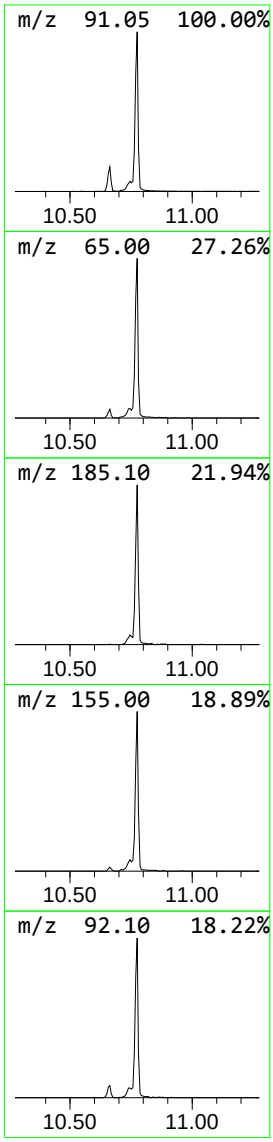
****
Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	7.50 ng	694272	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	N-Tosylethylenediamine	214	C9H14N2O2S	014316-16-6	59
3	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
4	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47





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Instrument :
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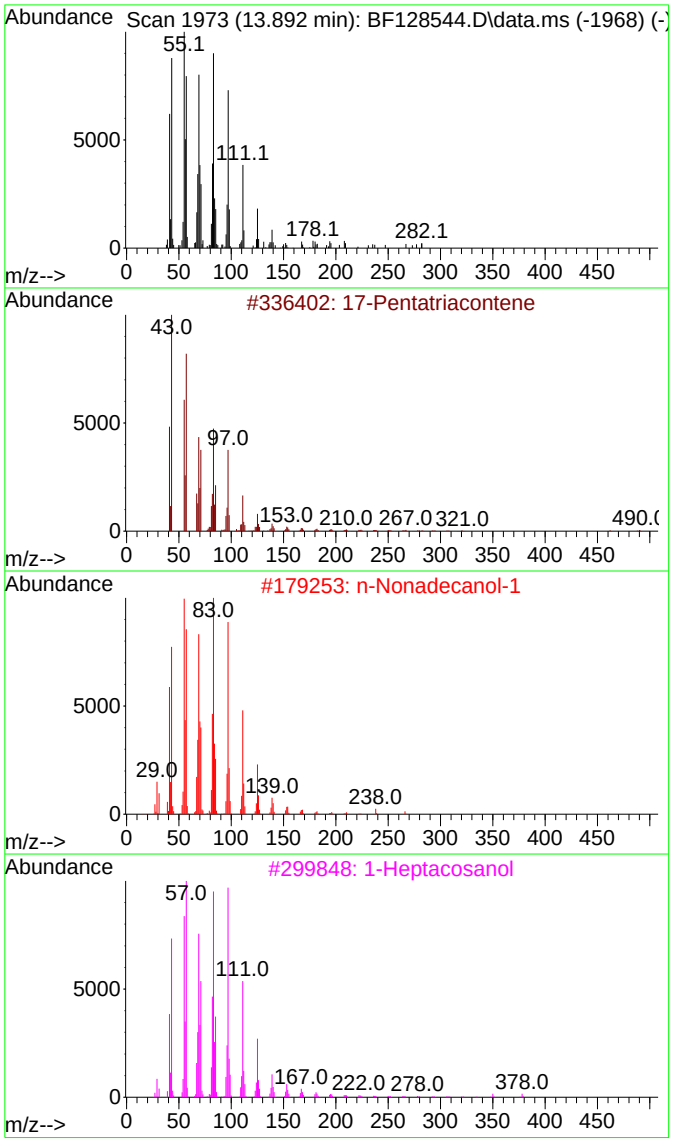
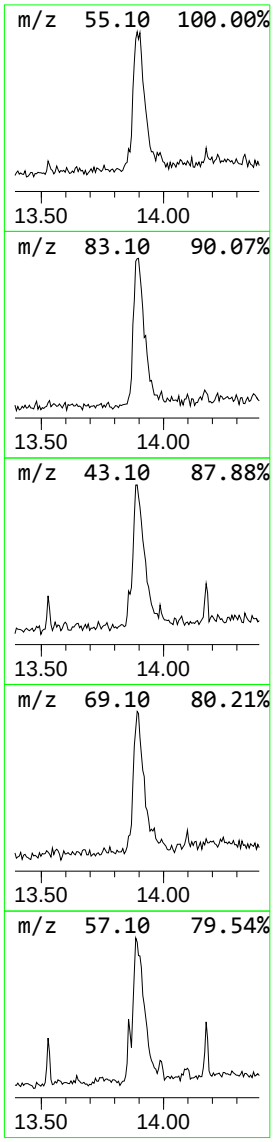
****

Peak Number 4 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.52 ng	372392	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	1-Octadecanol	270	C18H38O	000112-92-5	87
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83





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BNA_F
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TIC Library : C:\Database\NIST20.L
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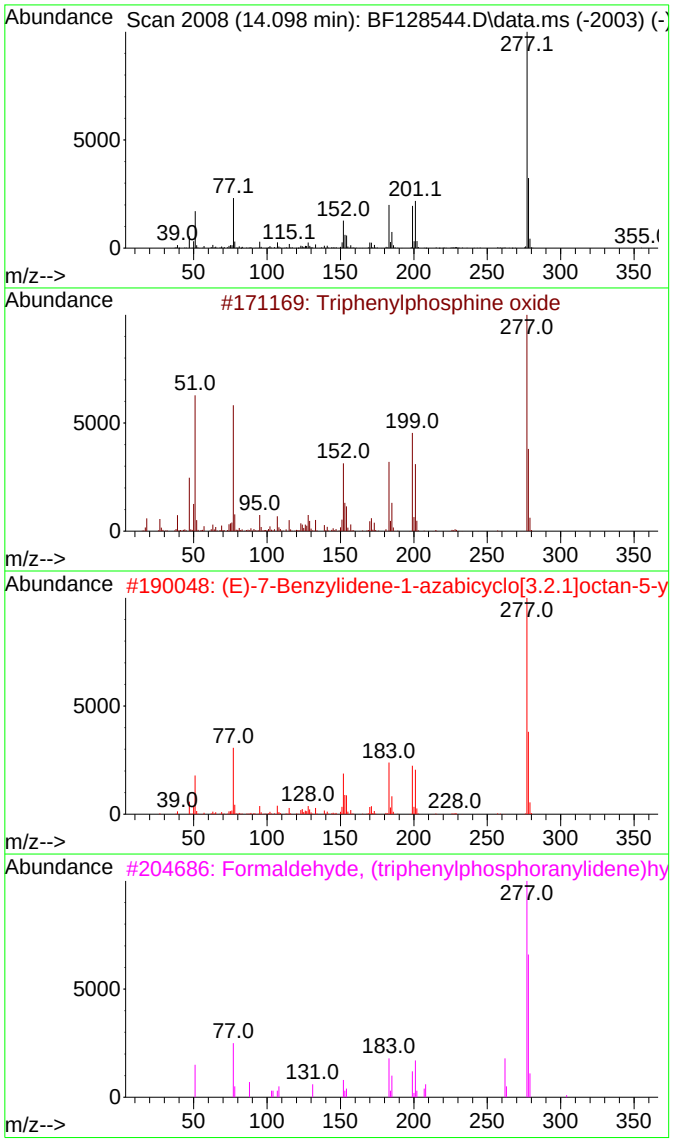
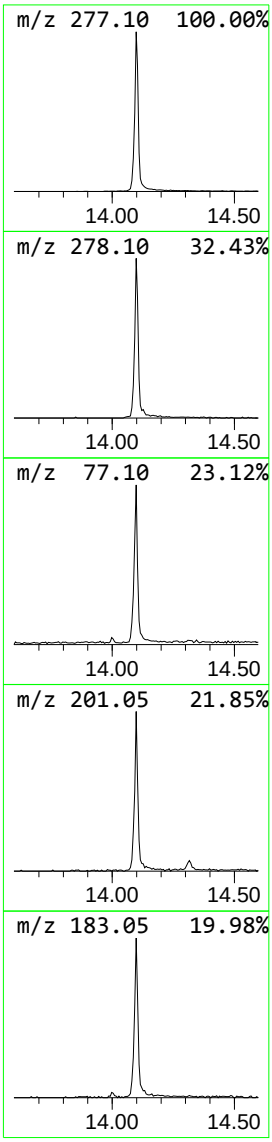
Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	7.21 ng	485858	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23





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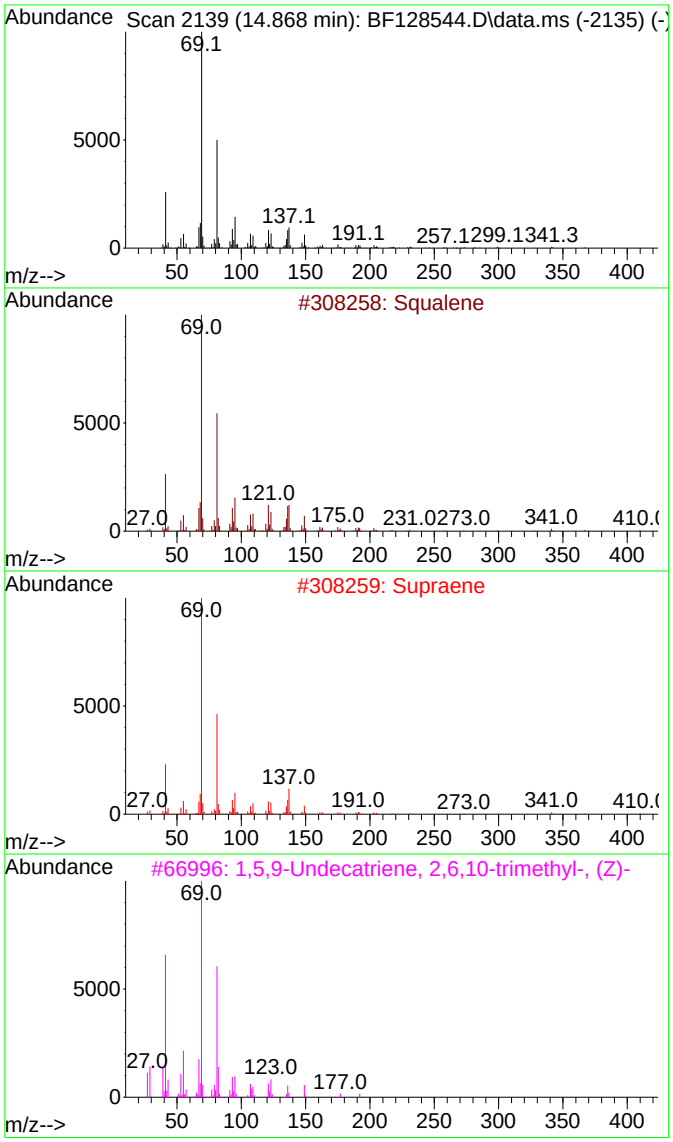
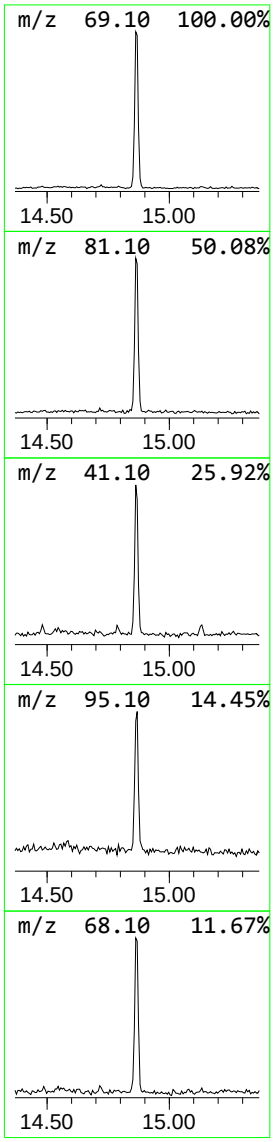
Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	6.55 ng	354668	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	78
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72





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-...	5.063	4.1	ng	240787	1	6.839	1167100	20.0
Benzenesulfonic...	9.822	7.9	ng	707918	3	9.875	1793720	20.0
Benzenesulfonam...	10.775	7.5	ng	694272	4	11.363	1851580	20.0
17-Pentatriacon...	13.892	5.5	ng	372392	5	14.004	1348330	20.0
Triphenylphosph...	14.098	7.2	ng	485858	5	14.004	1348330	20.0
Squalene	14.868	6.5	ng	354668	6	15.463	1082600	20.0