LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129908.D
Acq On : 19 Aug 2022 13:01
Operator : CG\JU
Sample : N4227-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129908.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	459	463	477	rBV	166078	216750	7.27%	1.073%
2	5.428	531	534	555	rBV	2372105	2434403	81.65%	12.048%
3	6.445	704	707	721	rBV	2510571	2423813	81.29%	11.995%
4	6.792	762	766	770	rBV	863320	690738	23.17%	3.418%
5	7.363	858	863	866	rBV	1672245	1568003	52.59%	7.760%
6	8.075	980	984	988	rBV	1147454	934495	31.34%	4.625%
7	9.151	1162	1167	1170	rBV	3475487	2981610	100.00%	14.756%
8	9.833	1279	1283	1286	rBV	1206706	1041551	34.93%	5.155%
9	10.627	1414	1418	1428	rBV	1973637	1629380	54.65%	8.064%
10	11.322	1533	1536	1540	rBV	1136774	941452	31.58%	4.659%
11	11.839	1619	1624	1629	rBV3	26178	36790	1.23%	0.182%
12	12.845	1788	1795	1797	rBV7	46713	95100	3.19%	0.471%
13	12.910	1799	1806	1809	rBV	2566616	2426774	81.39%	12.010%
14	12.992	1809	1820	1824	rVV4	174353	575474	19.30%	2.848%
15	13.804	1953	1958	1969	rBV4	46446	132256	4.44%	0.655%
16	13.974	1983	1987	1990	rBV	611166	573708	19.24%	2.839%
17	14.057	1997	2001	2007	rBV	144725	159356	5.34%	0.789%
18	15.039	2166	2168	2174	rVB	33127	40224	1.35%	0.199%
19	15.433	2218	2235	2246	rVB	558750	1099455	36.87%	5.441%
20	15.839	2300	2304	2310	rVB4	25898	38793	1.30%	0.192%
21	16.998	2495	2501	2507	rBV7	84332	166132	5.57%	0.822%

Sum of corrected areas: 20206257

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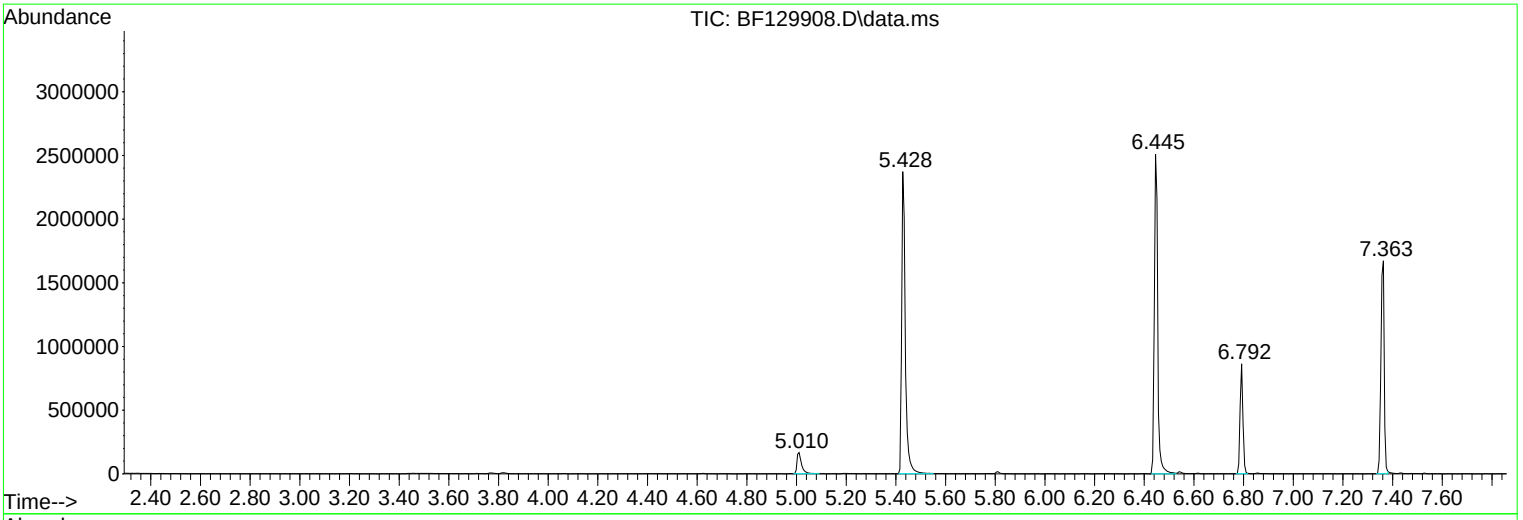
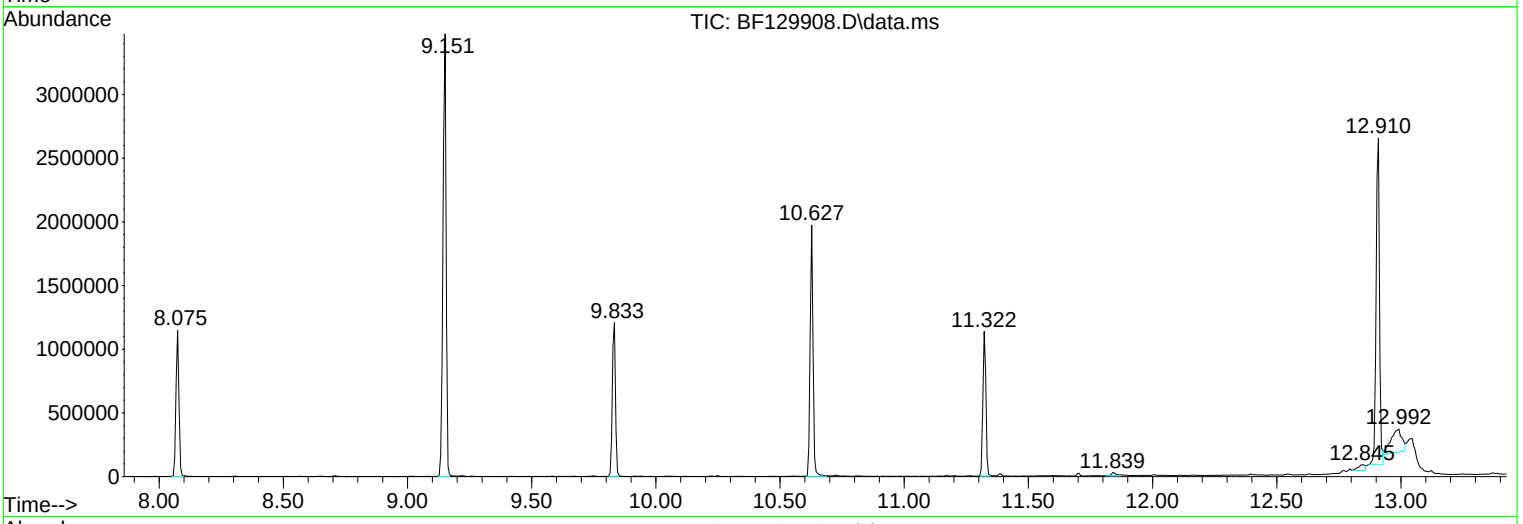
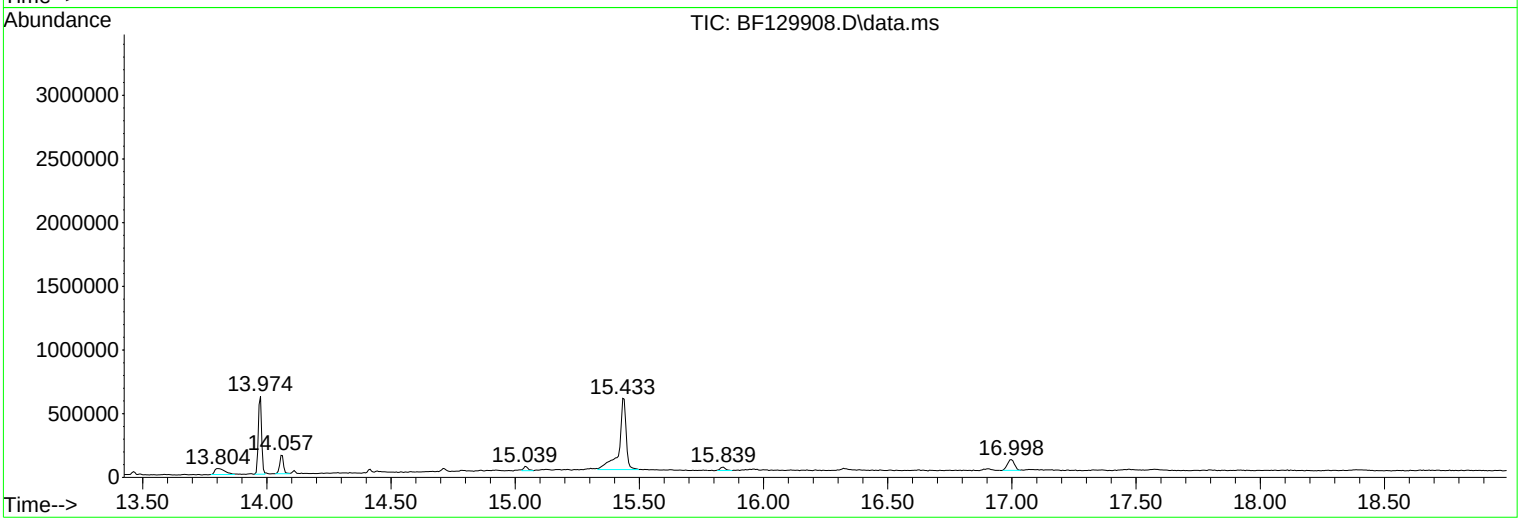
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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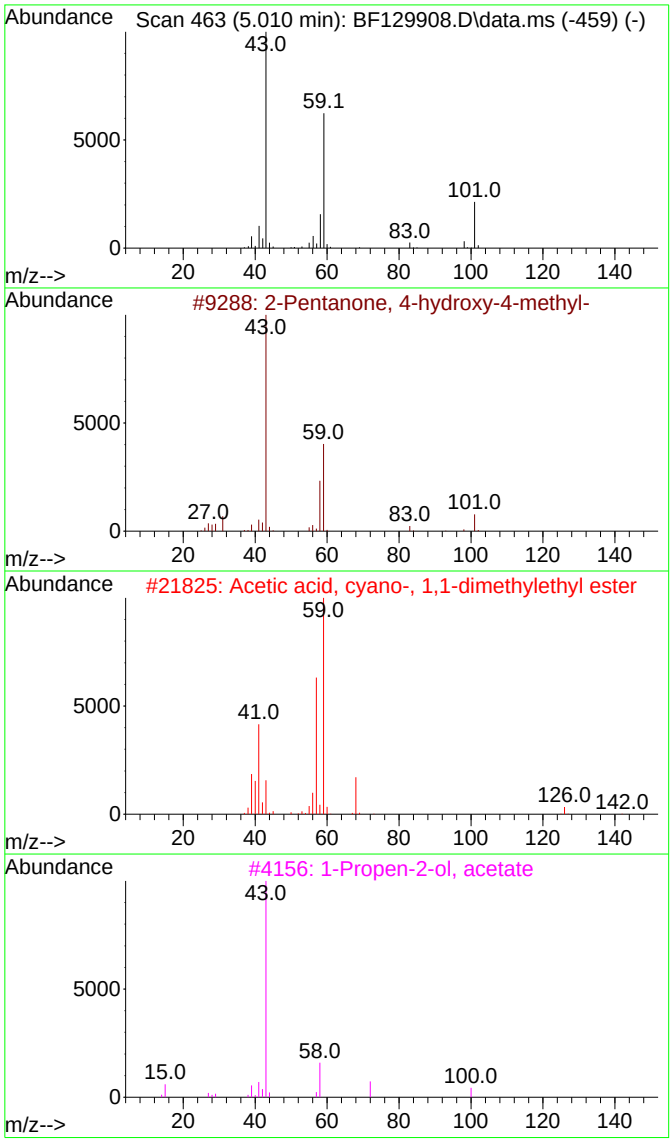
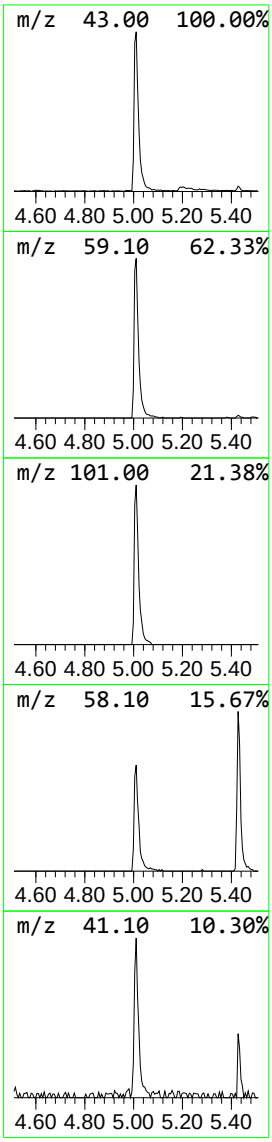
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	6.28 ng	216750	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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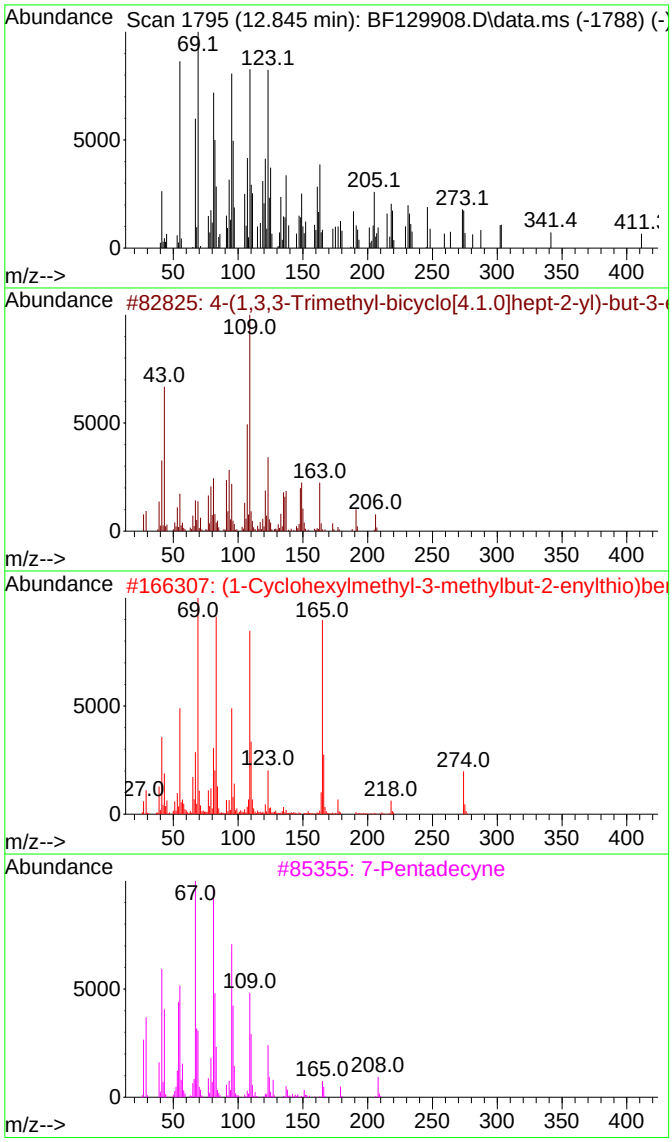
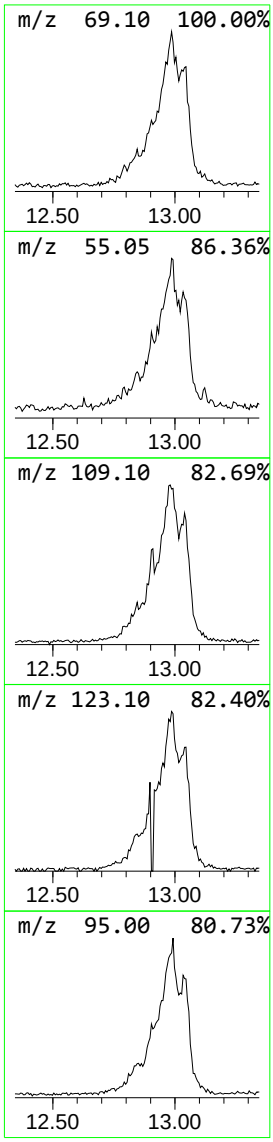
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4-(1,3,3-Trimethyl-bicyclo[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.845	3.32 ng	95100	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	70
2	(1-Cyclohexylmethyl-3-methylbut-...	274	C18H26S	1000191-26-0	38
3	7-Pentadecyne	208	C15H28	022089-89-0	25
4	2-[(3-Fluorophenyl)methyl]-5-([(...	328	C17H17FN4O2	1000386-81-0	22
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	20





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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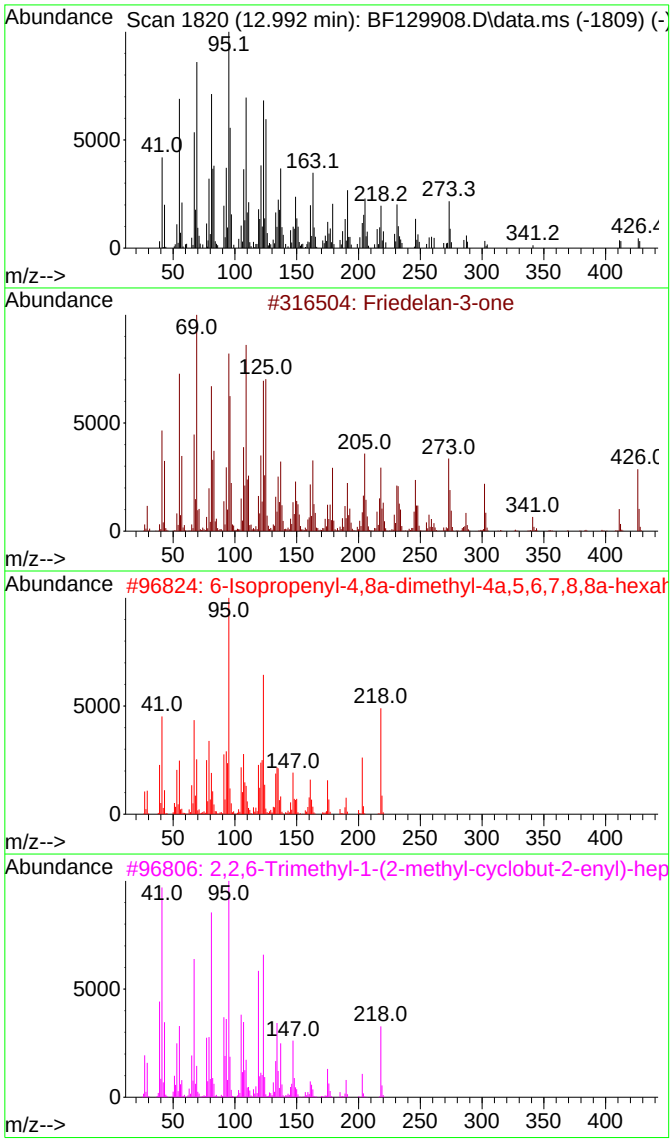
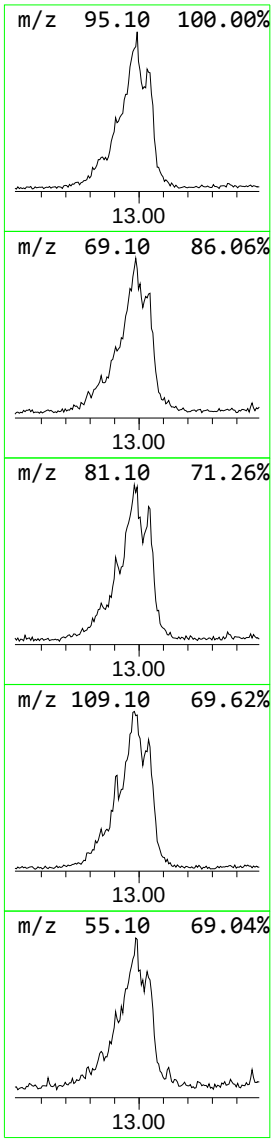
****

Peak Number 3 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	20.06 ng	575474	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	83
2	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	52
3	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	48
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	42
5	7-Tetradecyne	194	C14H26	035216-11-6	41





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
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TIC Library : C:\Database\NIST20.L
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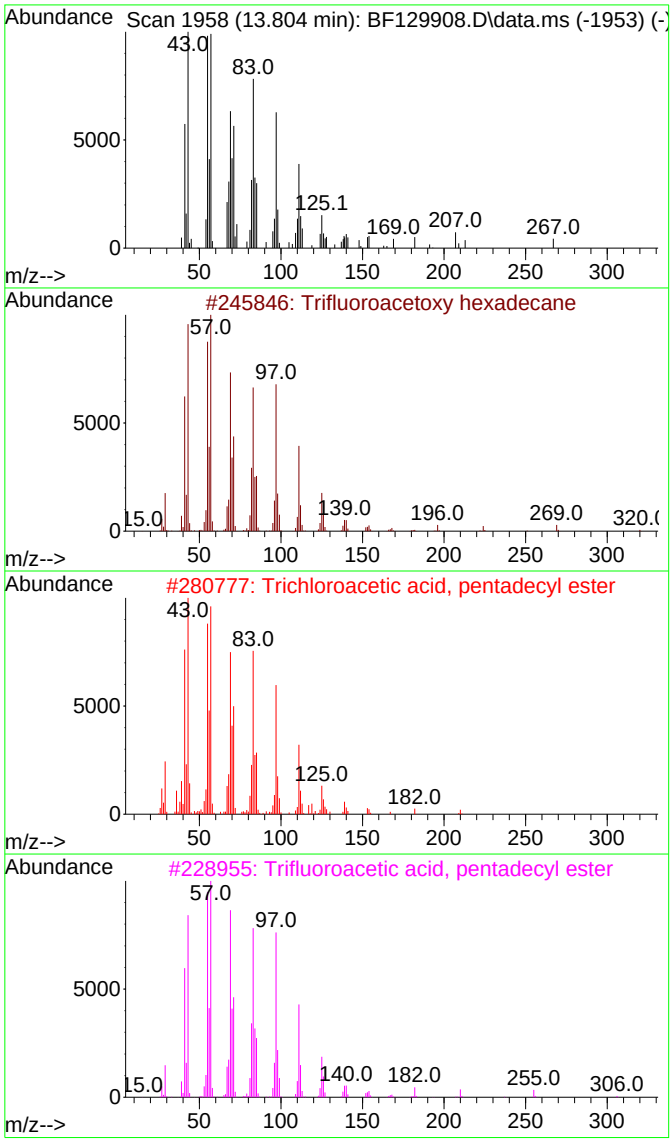
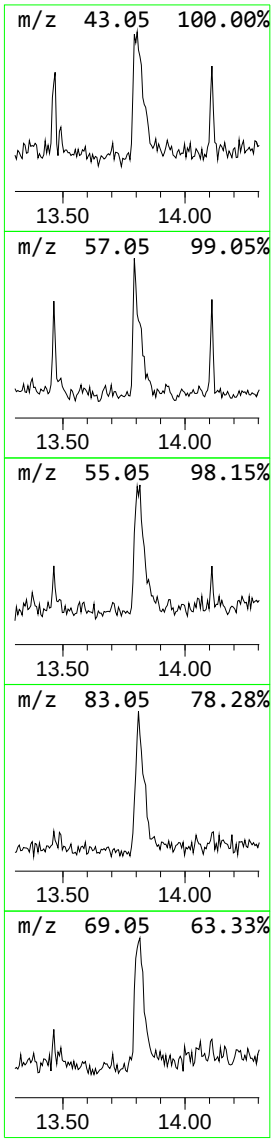
****

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	4.61 ng	132256	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93





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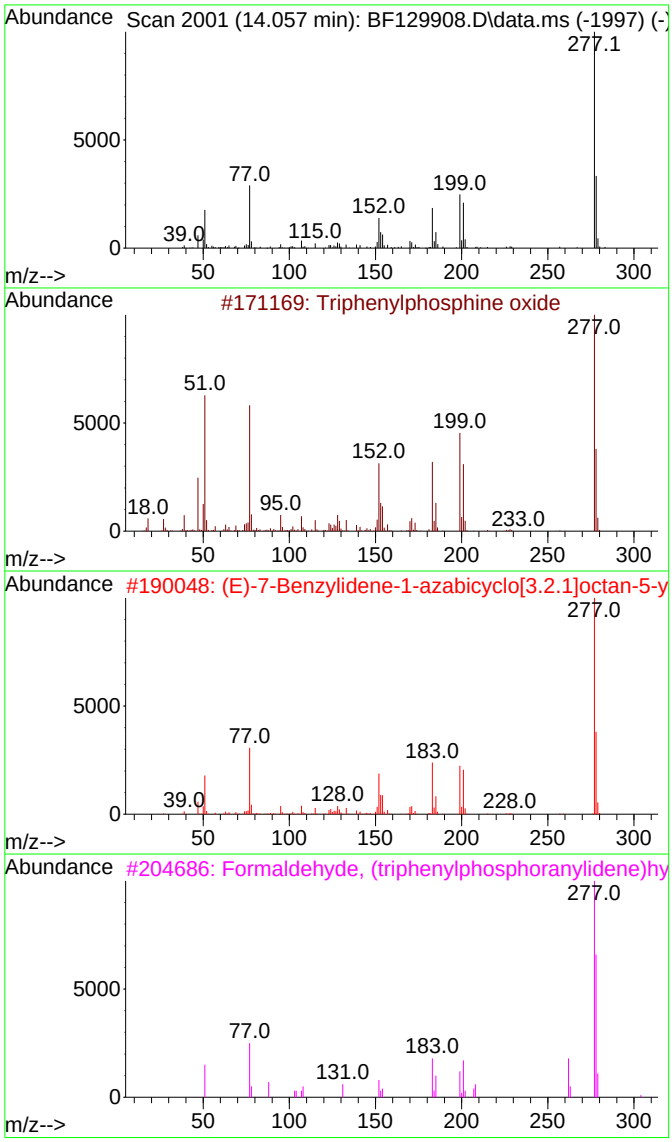
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

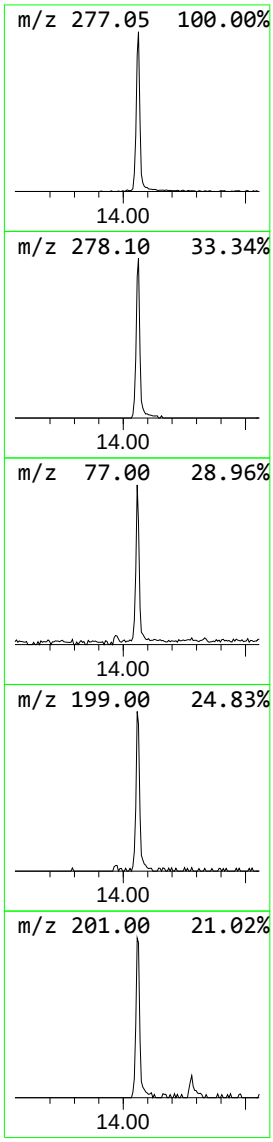
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	5.56 ng	159356	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	37
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	33





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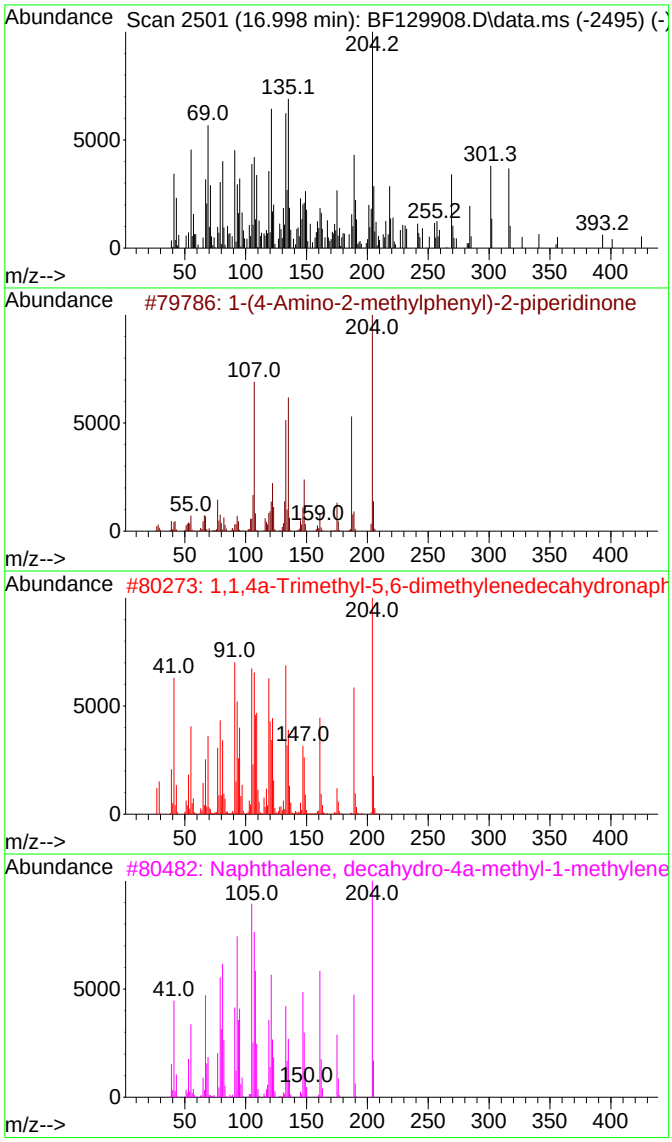
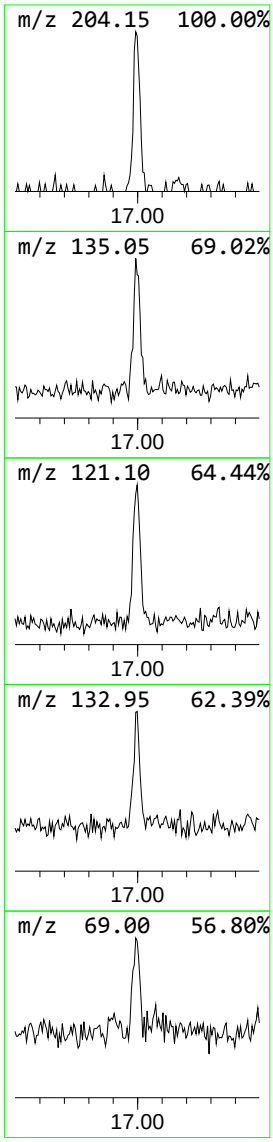
****
Peak Number 6 1-(4-Amino-2-methylphenyl)-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.998	3.02 ng	166132	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	58
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	52
3	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49
4	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	46
5	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	41





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-...	5.010	6.3	ng	216750	1	6.792	690738	20.0
4-(1,3,3-Trimet...	12.845	3.3	ng	95100	5	13.974	573708	20.0
Friedelan-3-one	12.992	20.1	ng	575474	5	13.974	573708	20.0
Trifluoroacetox...	13.804	4.6	ng	132256	5	13.974	573708	20.0
Triphenylphosph...	14.057	5.6	ng	159356	5	13.974	573708	20.0
1-(4-Amino-2-me...	16.998	3.0	ng	166132	6	15.439	1099460	20.0