

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061617\
 Data File : BF095960.D
 Acq On : 16 Jun 2017 17:37
 Operator : SJ/MA
 Sample : I3684-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROCKY-ROAD-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.504	492	496	511	rBV	47846	123633	7.26%	0.982%
2	5.216	613	617	651	rBV	531429	1224180	71.93%	9.721%
3	6.898	899	903	913	rBV	693760	1174782	69.03%	9.328%
4	6.981	913	917	932	rVB	927092	1529279	89.86%	12.143%
5	7.322	971	975	985	rBV	274812	366225	21.52%	2.908%
6	7.557	1010	1015	1035	rBV	792681	1071036	62.93%	8.505%
7	8.239	1127	1131	1149	rBV	558969	804652	47.28%	6.389%
8	9.351	1316	1320	1341	rBV	367251	507770	29.84%	4.032%
9	11.133	1617	1623	1639	rBV	1362100	1701903	100.00%	13.514%
10	11.827	1737	1741	1753	rBV	86170	118426	6.96%	0.940%
11	12.169	1795	1799	1806	rBV2	406816	539431	31.70%	4.283%
12	13.027	1940	1945	1950	rBV	19661	23198	1.36%	0.184%
13	13.468	2015	2020	2035	rBV	551194	807162	47.43%	6.409%
14	13.798	2071	2076	2083	rBV2	23370	30996	1.82%	0.246%
15	14.563	2202	2206	2221	rVB2	332579	472261	27.75%	3.750%
16	16.945	2606	2611	2619	rVB	1033503	1191374	70.00%	9.460%
17	17.615	2719	2725	2730	rBV	35028	43113	2.53%	0.342%
18	17.792	2752	2755	2759	rVB	20496	20142	1.18%	0.160%
19	18.209	2821	2826	2835	rBV3	53856	90916	5.34%	0.722%
20	18.292	2835	2840	2849	rBV	257281	340237	19.99%	2.702%
21	18.615	2890	2895	2900	rBV	26664	30143	1.77%	0.239%
22	18.998	2956	2960	2970	rBV2	15789	22082	1.30%	0.175%
23	19.956	3119	3123	3136	rBV2	265401	360607	21.19%	2.863%

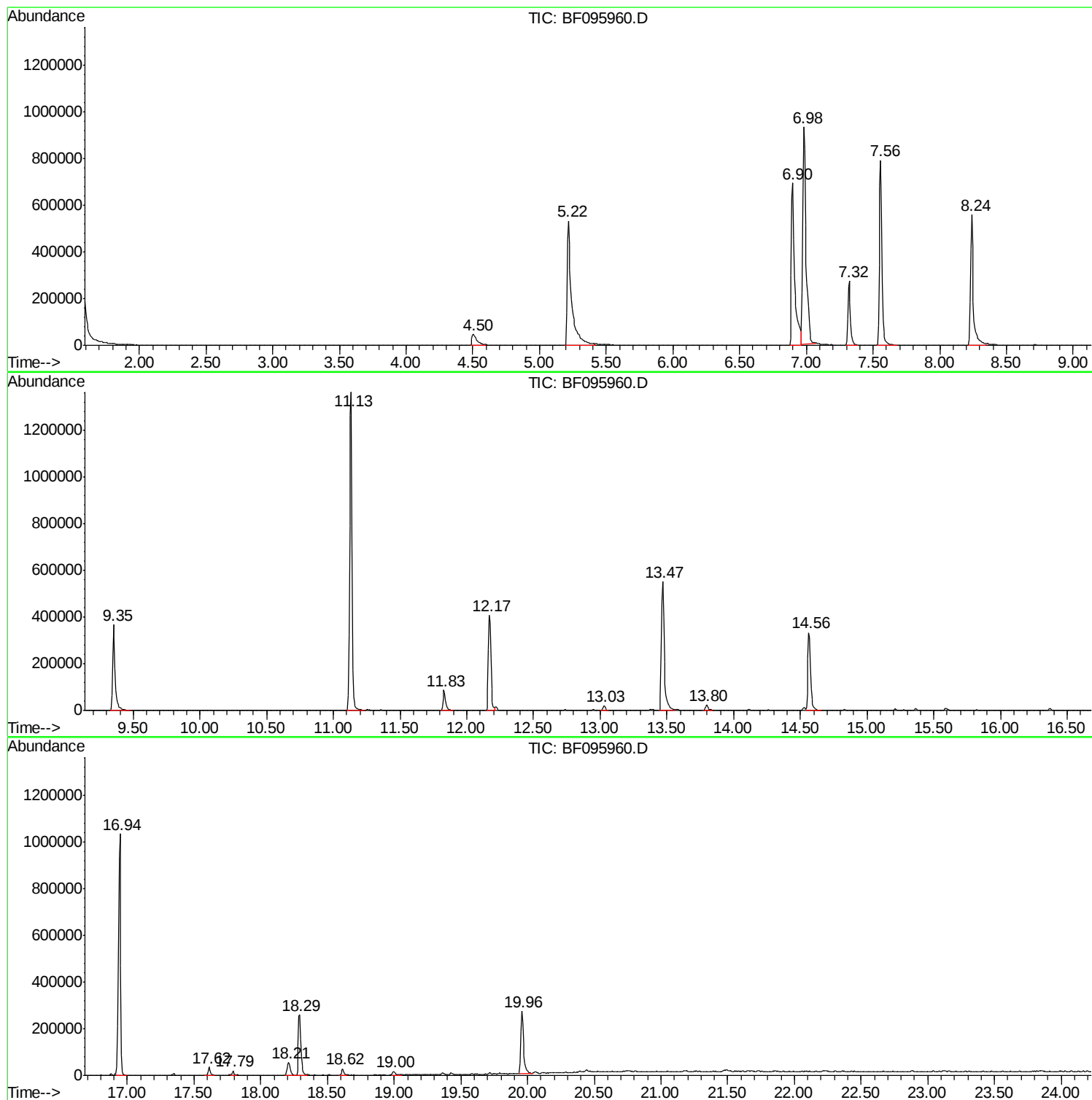
Sum of corrected areas: 12593548

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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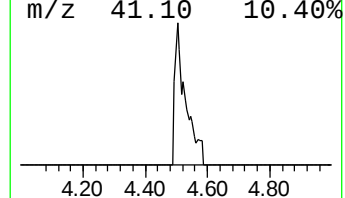
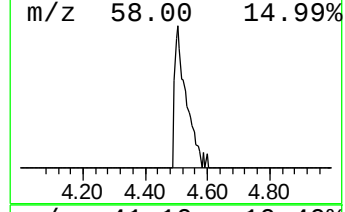
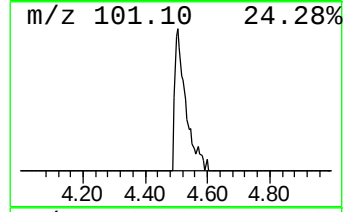
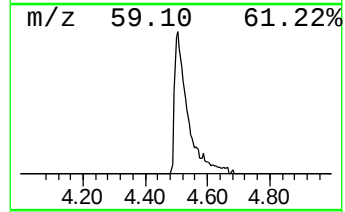
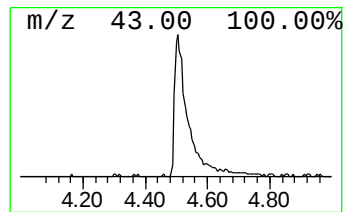
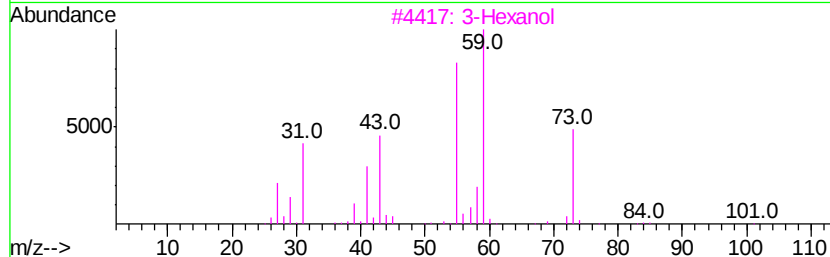
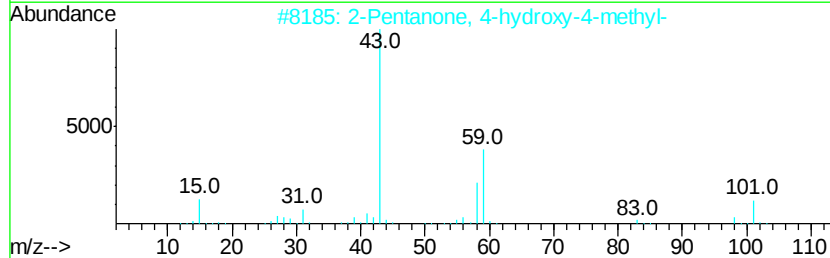
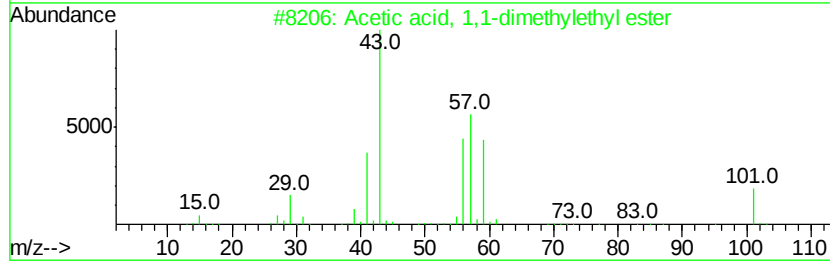
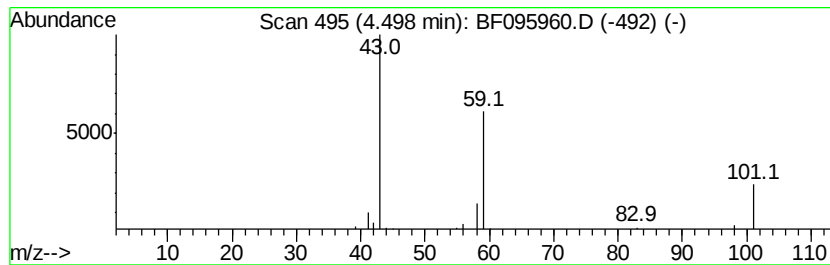
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.50 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	6.75 ng	123633	1,4-Dichlorobenzene-d4	7.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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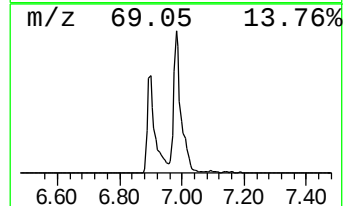
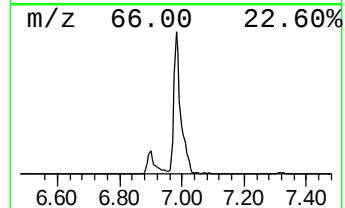
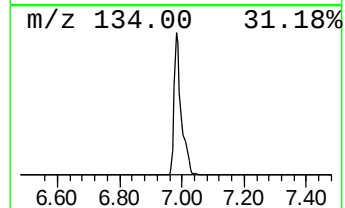
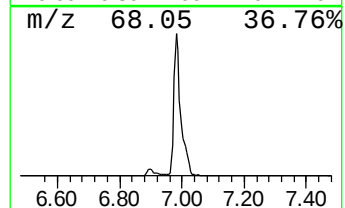
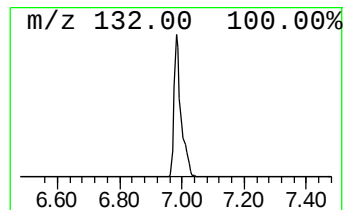
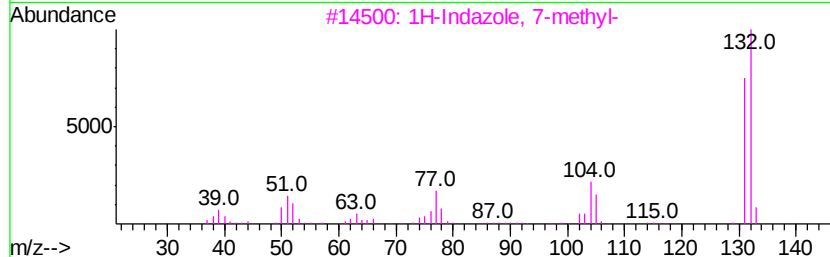
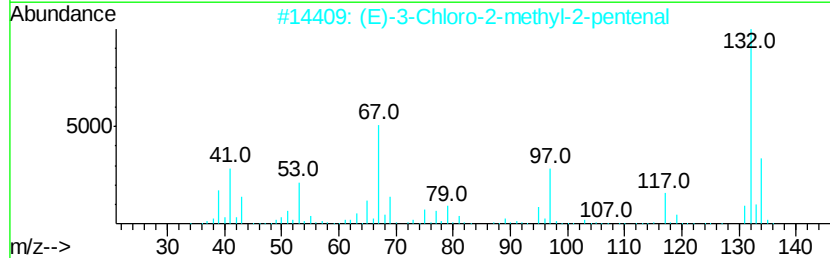
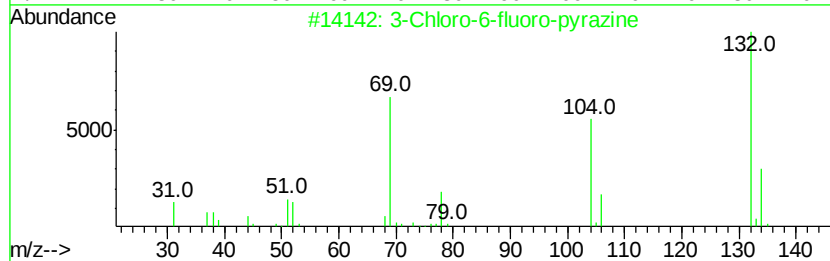
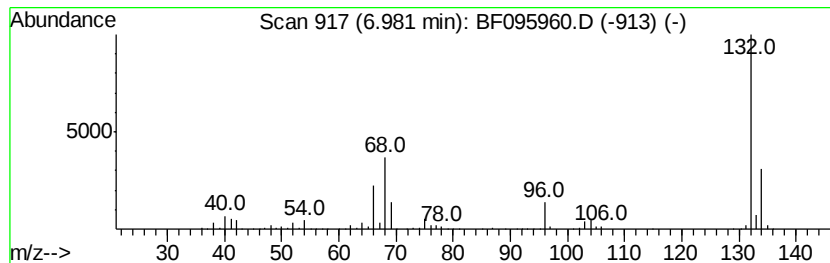
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Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	83.52 ng	1529280	1,4-Dichlorobenzene-d4	7.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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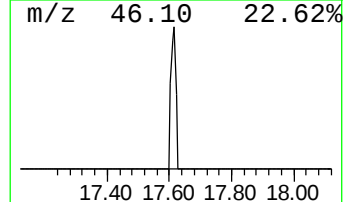
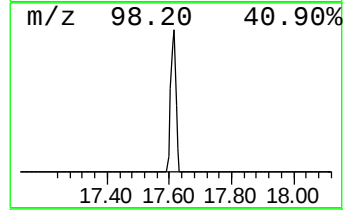
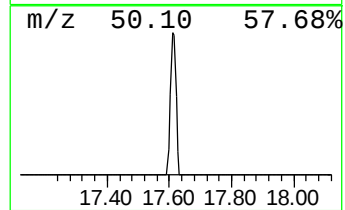
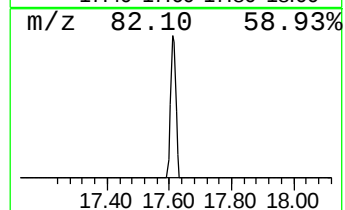
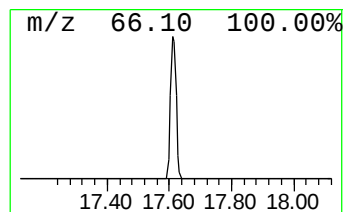
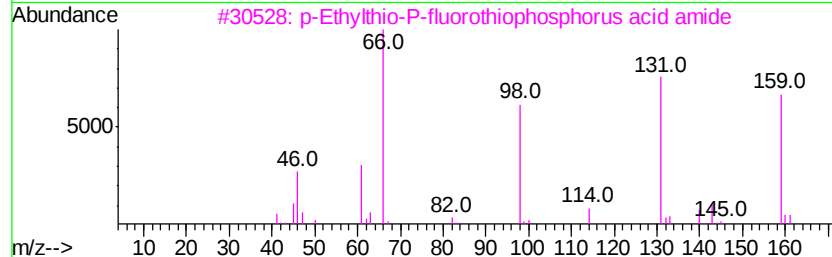
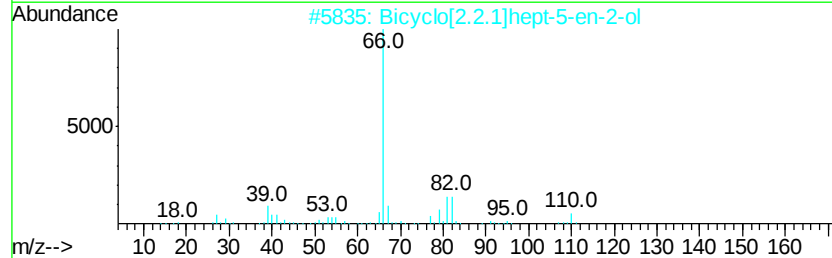
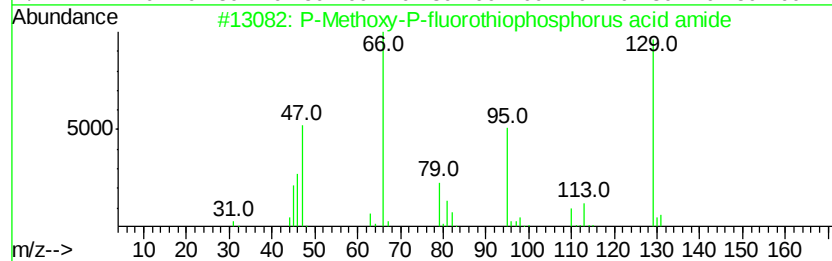
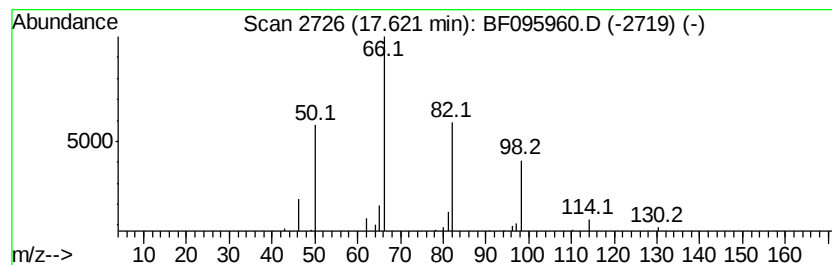
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Peak Number 4 unknown17.62 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.53 ng	43113	Chrysene-d12	18.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	P-Methoxy-P-fluorothiophosphorus...	129	CH5FNOPS	1000311-29-8	32
2		Bicyclo[2.2.1]hept-5-en-2-ol	110	C7H10O	013080-90-5	25
3		p-Ethylthio-P-fluorothiophosphor...	159	C2H7FNPS2	1000311-29-9	25
4		4-Pyridinamine, 3-nitro-	139	C5H5N3O2	001681-37-4	23
5		1-Buten-3-yne, 2-methyl-	66	C5H6	000078-80-8	23



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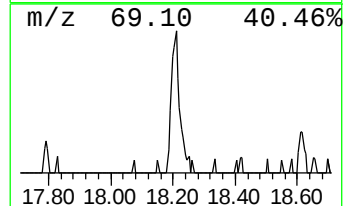
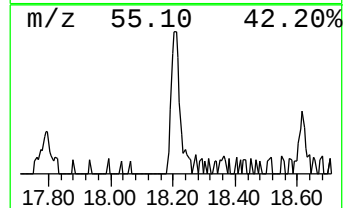
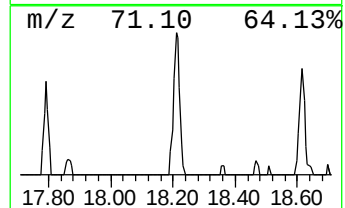
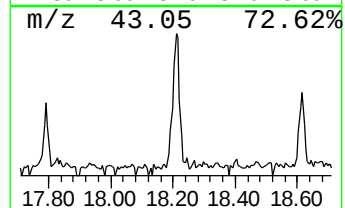
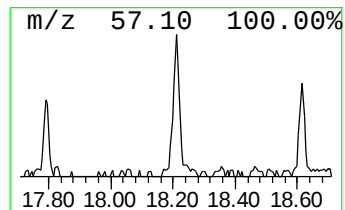
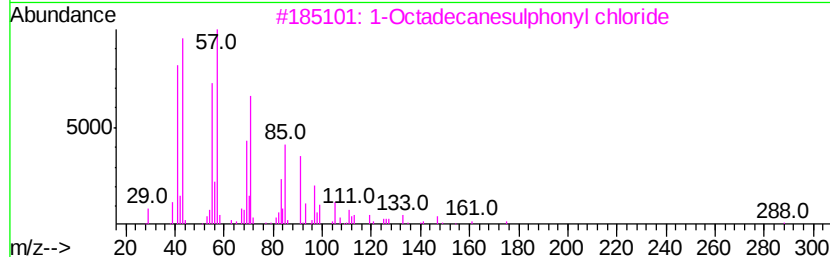
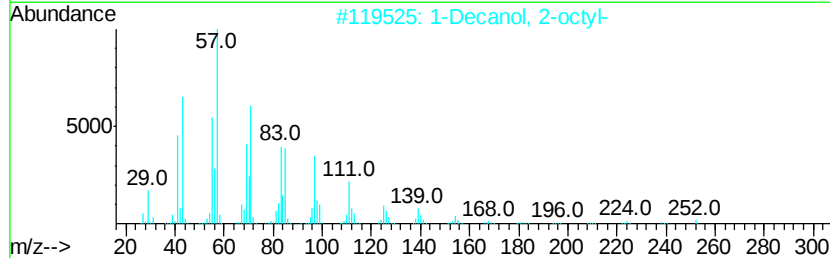
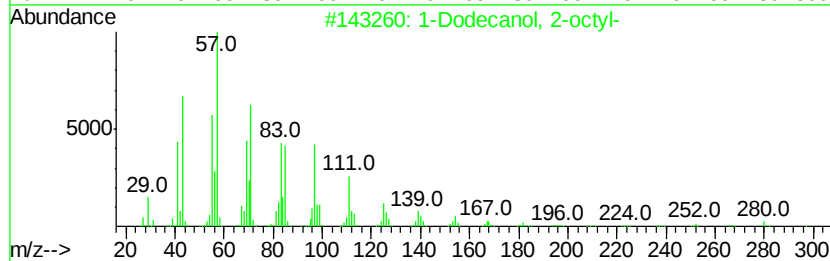
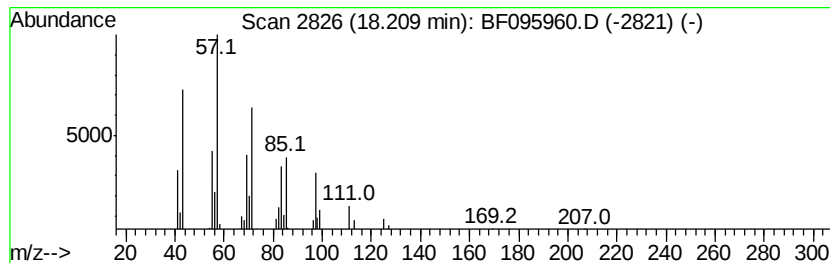
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Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.21	5.34 ng	90916	Chrysene-d12	18.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	90
3	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
4	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	86
5	Hexatriacontyl trifluoroacetate	619	C38H73F3O2	1000351-88-6	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.50	4.50	6.8	ng	123633	1	7.32	366225	20.0
unknown6.98	6.98	83.5	ng	1529280	1	7.32	366225	20.0
unknown17.62	17.62	2.5	ng	43113	5	18.29	340237	20.0
1-Dodecanol, 2-oc...	18.21	5.3	ng	90916	5	18.29	340237	20.0