

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081822\
 Data File : BF129890.D
 Acq On : 18 Aug 2022 22:54
 Operator : CG\JU
 Sample : N4215-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-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: BF129890.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	460	463	477	rBV	112270	142786	5.14%	0.740%
2	5.428	530	534	554	rBV	2592944	2485842	89.55%	12.887%
3	6.445	703	707	721	rBV	2890238	2524165	90.93%	13.085%
4	6.792	762	766	773	rVB	768503	673630	24.27%	3.492%
5	7.357	858	862	872	rBV	1797900	1595247	57.47%	8.270%
6	8.075	980	984	987	rBV	985590	891680	32.12%	4.622%
7	9.145	1162	1166	1170	rBV	3051925	2775805	100.00%	14.390%
8	9.828	1278	1282	1286	rBV	1121044	945799	34.07%	4.903%
9	10.622	1413	1417	1428	rBV	1602384	1453223	52.35%	7.534%
10	11.322	1532	1536	1538	rBV	931954	784021	28.24%	4.064%
11	11.345	1538	1540	1544	rVB	59103	48163	1.74%	0.250%
12	11.698	1597	1600	1604	rVB	80440	61971	2.23%	0.321%
13	11.851	1622	1626	1633	rVB3	21774	36429	1.31%	0.189%
14	12.539	1738	1743	1748	rBV	88833	83908	3.02%	0.435%
15	12.769	1776	1782	1787	rBV	97673	100441	3.62%	0.521%
16	12.904	1801	1805	1808	rBV	2054575	1715881	61.82%	8.895%
17	13.804	1951	1958	1971	rBV9	37757	132088	4.76%	0.685%
18	13.968	1981	1986	1989	rBV	656301	622518	22.43%	3.227%
19	13.992	1989	1990	1994	rVB	55567	42517	1.53%	0.220%
20	14.057	1996	2001	2008	rBV	303352	316423	11.40%	1.640%
21	14.704	2107	2111	2119	rBV	885440	848674	30.57%	4.400%
22	15.004	2158	2162	2166	rBV	56137	88448	3.19%	0.459%
23	15.304	2210	2213	2219	rVB	32716	43060	1.55%	0.223%
24	15.368	2221	2224	2228	rBV	43305	50960	1.84%	0.264%
25	15.427	2229	2234	2244	rVB	585024	734525	26.46%	3.808%
26	16.898	2480	2484	2491	rVB3	30830	55940	2.02%	0.290%
27	17.345	2556	2560	2567	rVB2	18171	36000	1.30%	0.187%

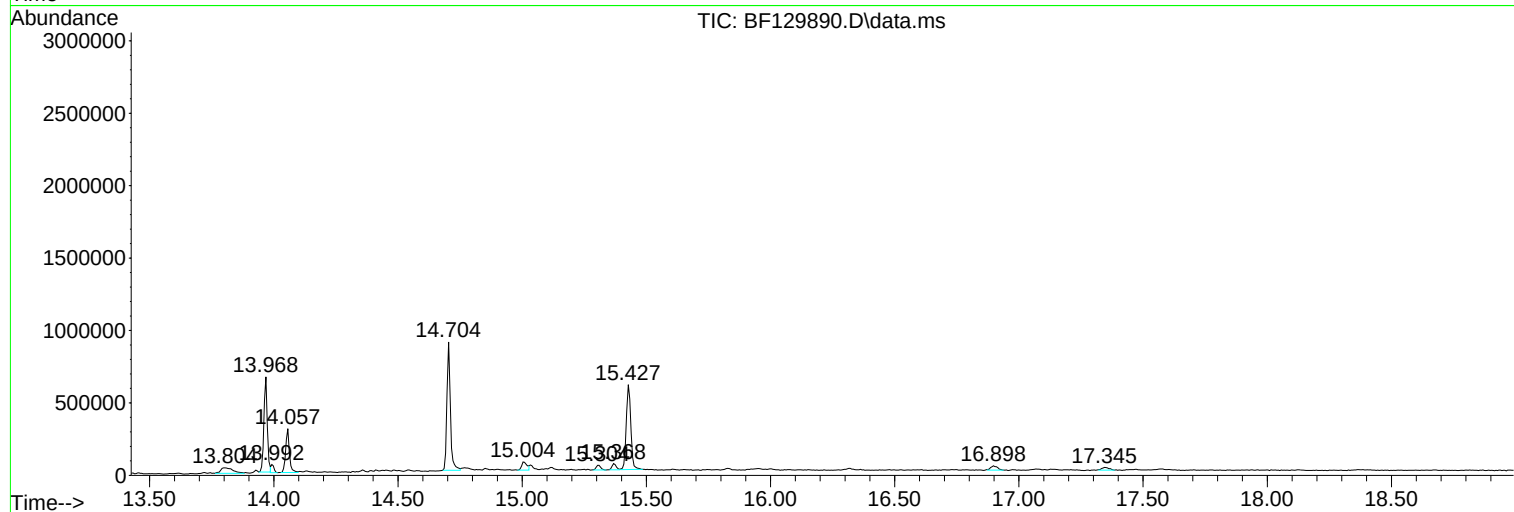
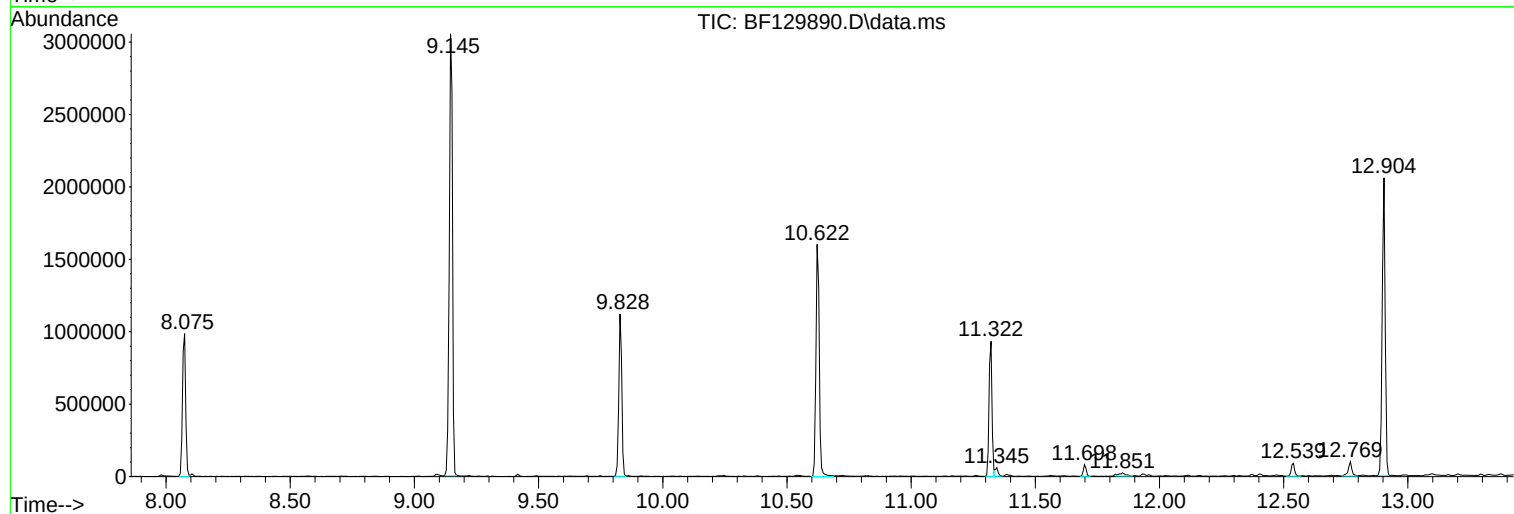
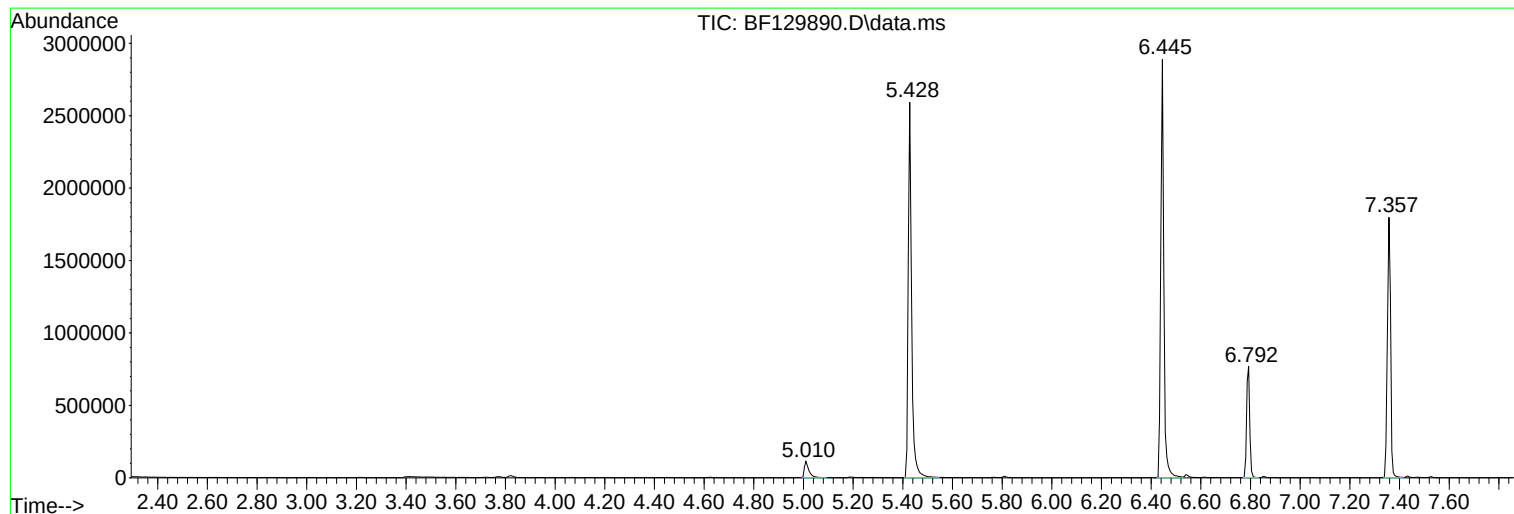
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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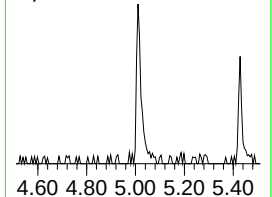
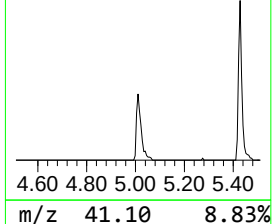
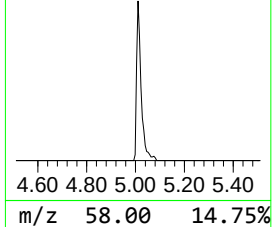
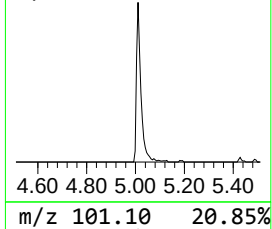
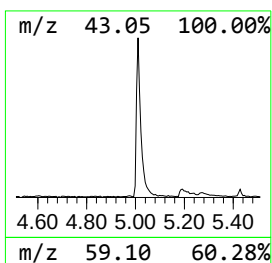
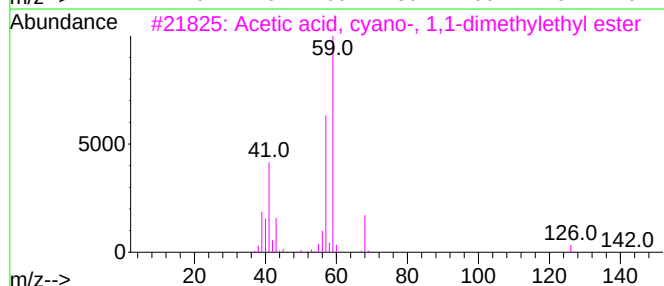
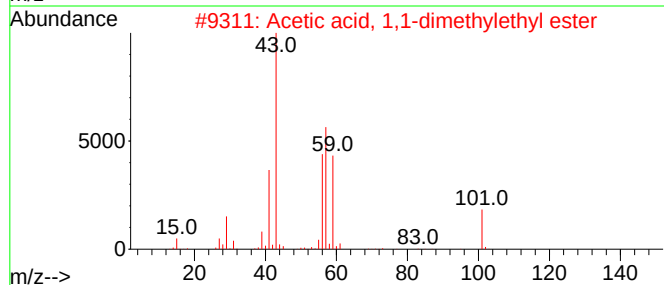
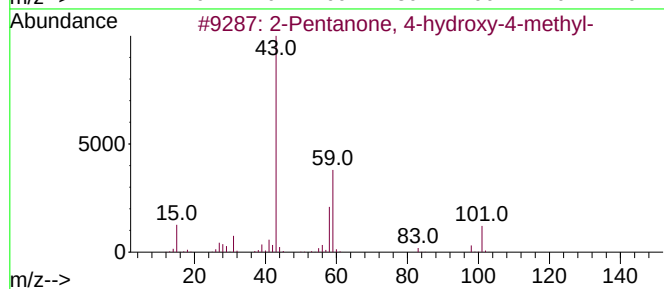
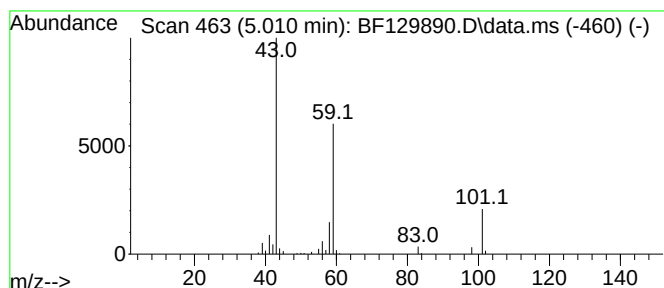
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	4.24 ng	142786	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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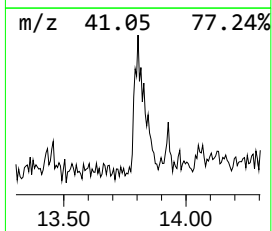
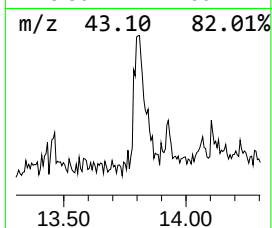
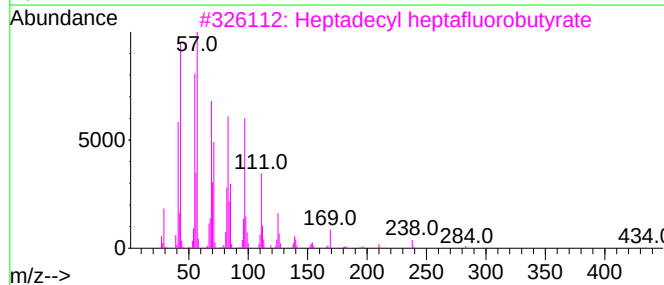
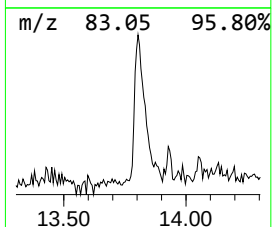
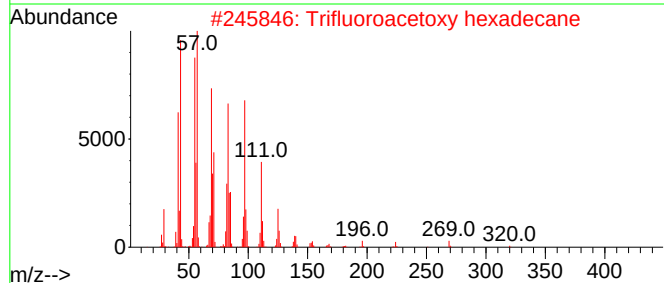
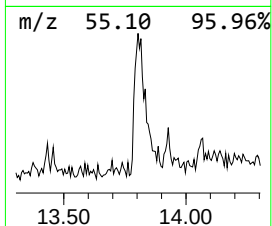
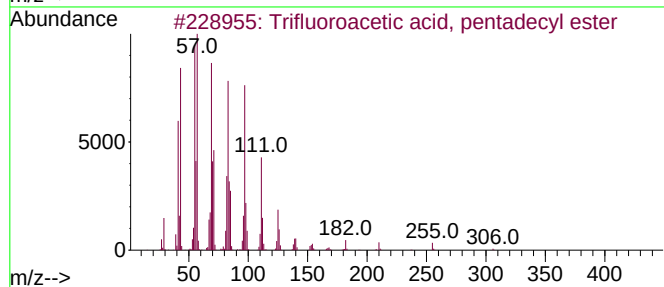
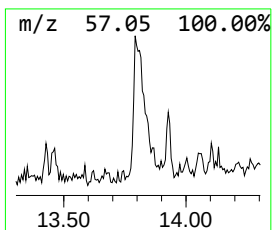
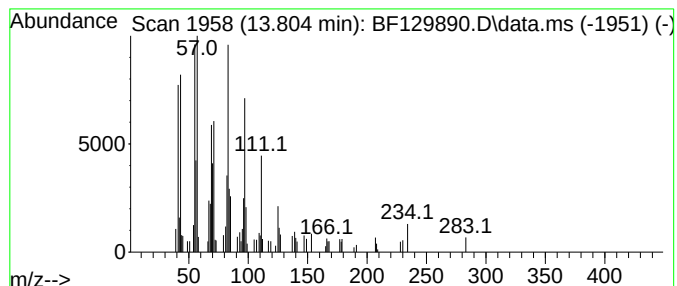
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Trifluoroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	4.24 ng	132088	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5			1-Docosene	308	C22H44	001599-67-3	87



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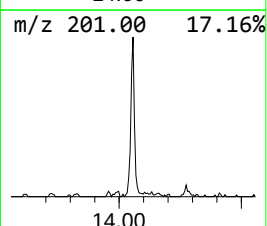
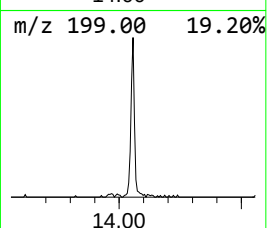
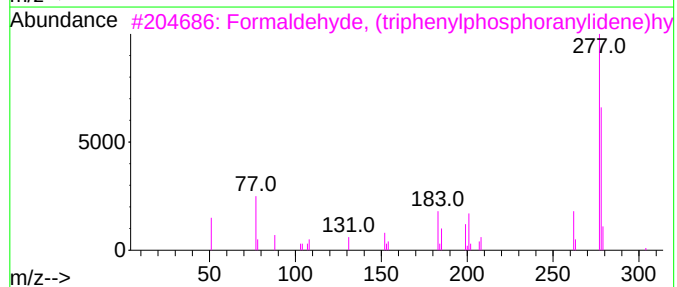
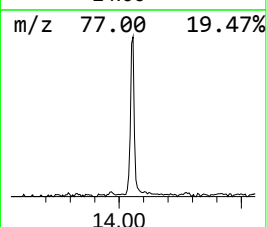
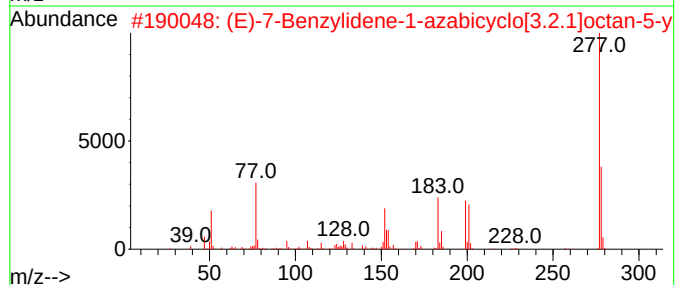
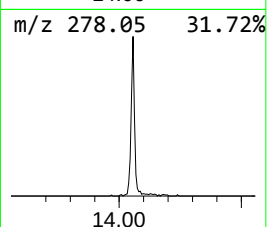
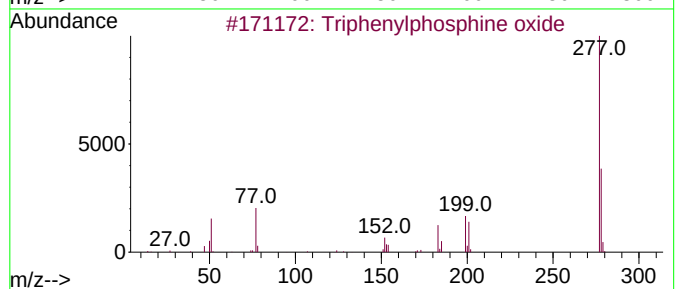
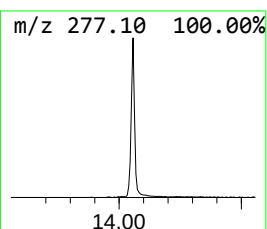
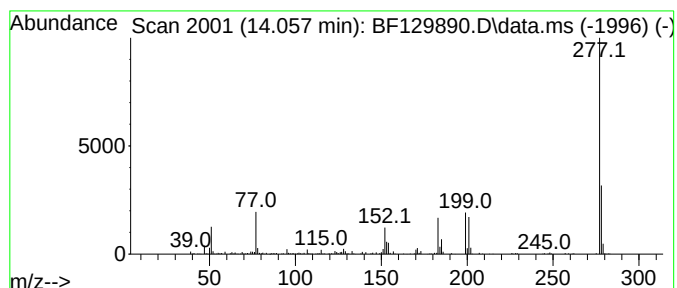
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	10.17 ng	316423	Chrysene-d12	13.968

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	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33



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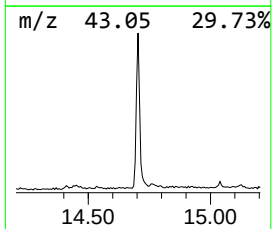
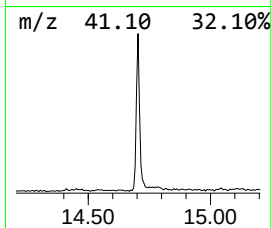
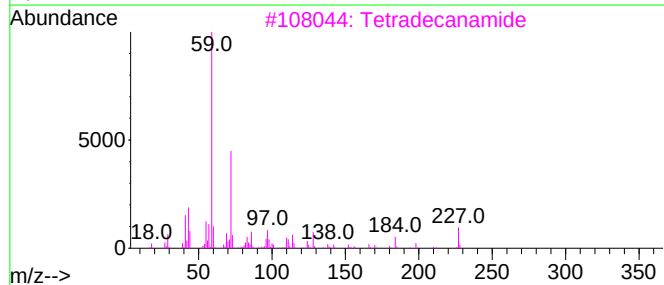
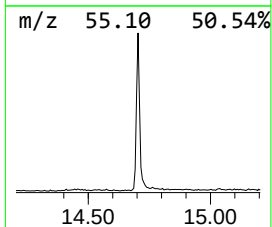
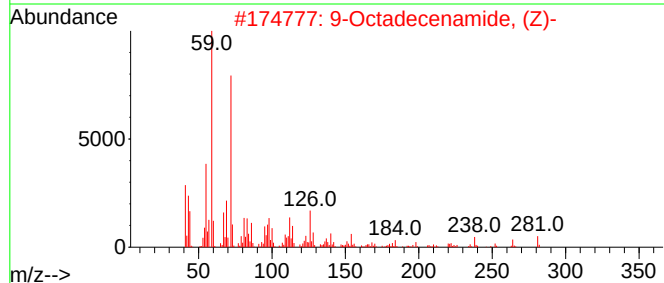
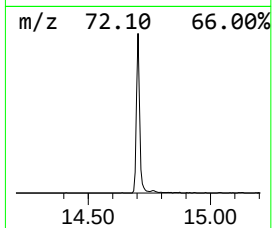
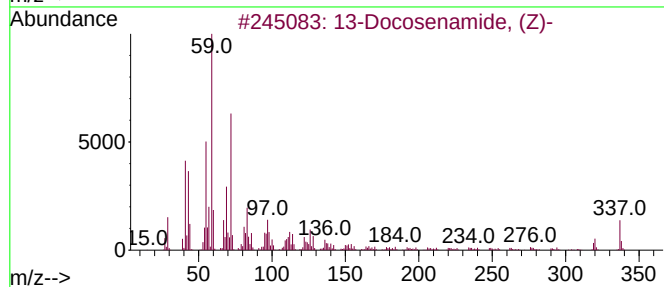
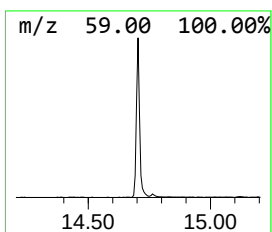
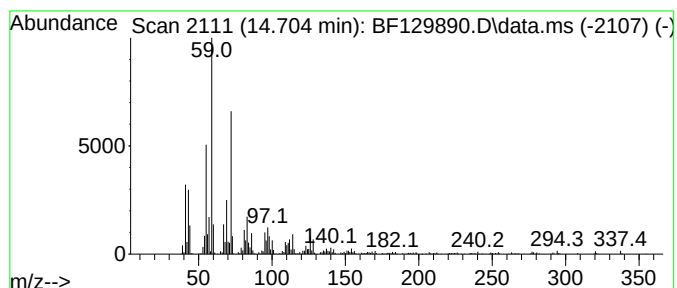
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	23.11 ng	848674	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3			Tetradecanamide	227	C14H29NO	000638-58-4	78
4			Palmitoleamide	253	C16H31NO	106010-22-4	64
5			Dodecanamide	199	C12H25NO	001120-16-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.010	4.2	ng	142786	1	6.792	673630	20.0
Trifluoroacetic...	13.804	4.2	ng	132088	5	13.968	622518	20.0
Triphenylphosph...	14.057	10.2	ng	316423	5	13.968	622518	20.0
13-Docosenamide...	14.704	23.1	ng	848674	6	15.427	734525	20.0