

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013125\
 Data File : BF141350.D
 Acq On : 31 Jan 2025 23:37
 Operator : RC/JU
 Sample : Q1194-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-110-SB02

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-BF012925.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	4	10	22	rVB	59286	97211	3.63%	0.470%
2	5.004	490	495	504	rVB	35582	55478	2.07%	0.269%
3	5.422	560	566	585	rBV	1828388	2543144	95.07%	12.308%
4	5.981	656	661	668	rBV	18356	26825	1.00%	0.130%
5	6.440	733	739	760	rVB	1747970	2560707	95.72%	12.393%
6	6.798	795	800	805	rBV	746852	910293	34.03%	4.406%
7	7.357	889	895	900	rBV	1275670	1623521	60.69%	7.857%
8	7.616	933	939	945	rBV	60043	75587	2.83%	0.366%
9	8.081	1012	1018	1023	rBV	968117	1205587	45.07%	5.835%
10	8.298	1047	1055	1064	rBV2	26077	39732	1.49%	0.192%
11	9.157	1195	1201	1206	rBV	2080955	2675103	100.00%	12.947%
12	9.298	1221	1225	1238	rVB2	14270	28305	1.06%	0.137%
13	9.834	1311	1316	1329	rBV	1057602	1315880	49.19%	6.369%
14	10.545	1433	1437	1445	rBV	121589	161615	6.04%	0.782%
15	10.622	1445	1450	1461	rBV	1119682	1465773	54.79%	7.094%
16	11.322	1564	1569	1575	rVB	884623	1105615	41.33%	5.351%
17	11.857	1655	1660	1683	rBV2	93595	216106	8.08%	1.046%
18	12.645	1789	1794	1805	rBV10	11570	28622	1.07%	0.139%
19	12.910	1833	1839	1844	rBV	1441850	1814580	67.83%	8.782%
20	13.457	1926	1932	1936	rBV	277474	371571	13.89%	1.798%
21	13.498	1936	1939	1945	rVB2	36623	53361	1.99%	0.258%
22	13.604	1953	1957	1962	rBV	25897	35501	1.33%	0.172%
23	13.698	1968	1973	1976	rBV2	25010	37251	1.39%	0.180%
24	13.792	1985	1989	1992	rBV	23767	34952	1.31%	0.169%
25	13.869	1997	2002	2011	rVV5	36652	96260	3.60%	0.466%
26	13.963	2012	2018	2026	rVB	648027	872438	32.61%	4.222%
27	14.263	2064	2069	2078	rBV2	15693	33487	1.25%	0.162%
28	14.345	2079	2083	2089	rBV6	21839	30361	1.13%	0.147%
29	14.445	2095	2100	2104	rBV	36437	50161	1.88%	0.243%
30	14.504	2106	2110	2122	rVV10	8736	31005	1.16%	0.150%
31	15.080	2203	2208	2214	rBV	60933	89710	3.35%	0.434%
32	15.416	2260	2265	2279	rVB	479146	768196	28.72%	3.718%
33	15.892	2341	2346	2356	rVB	28518	55379	2.07%	0.268%
34	16.739	2484	2490	2500	rVB2	45399	90729	3.39%	0.439%
35	18.221	2736	2742	2751	rVB7	24674	62034	2.32%	0.300%

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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-BF012925.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

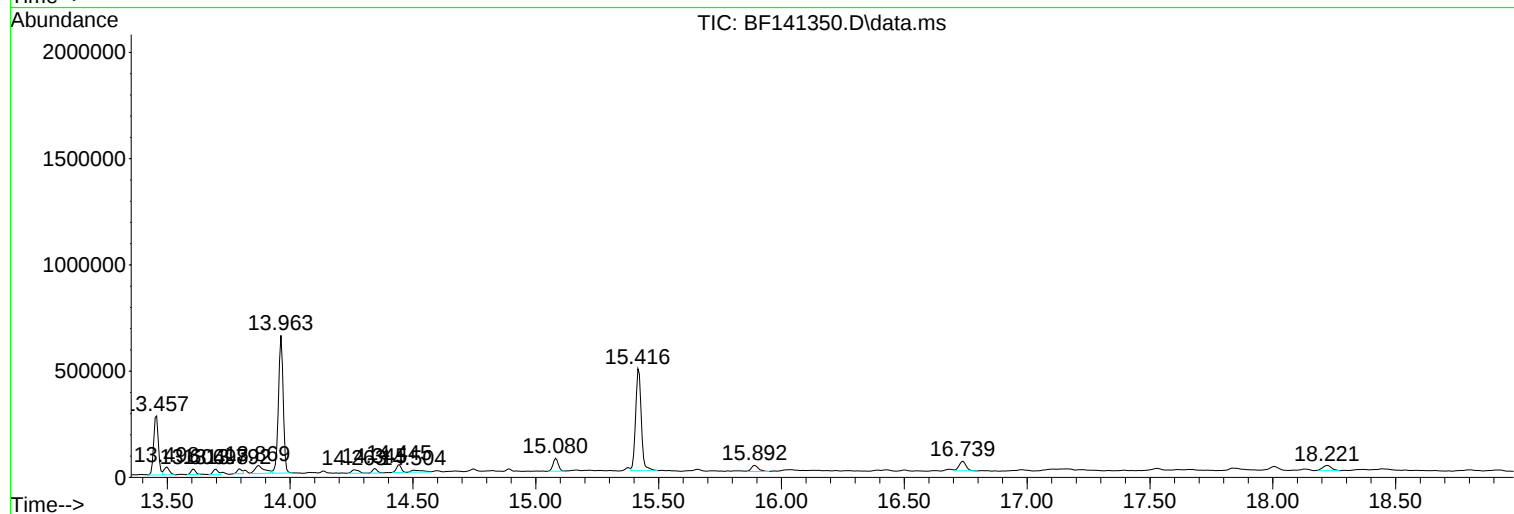
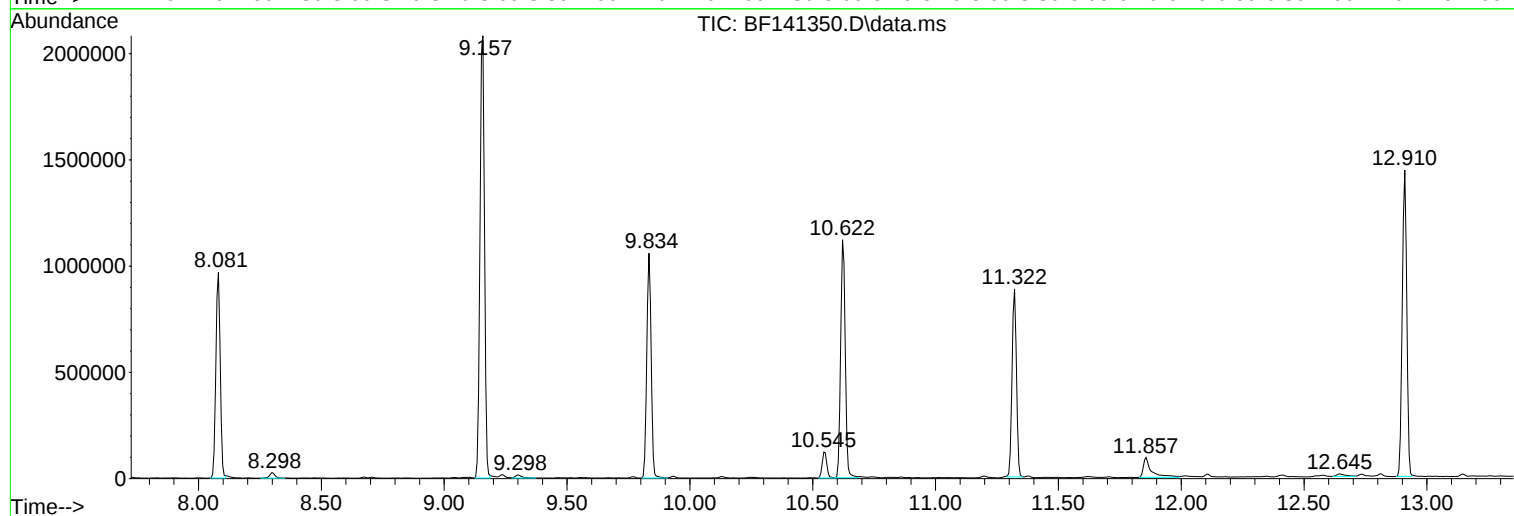
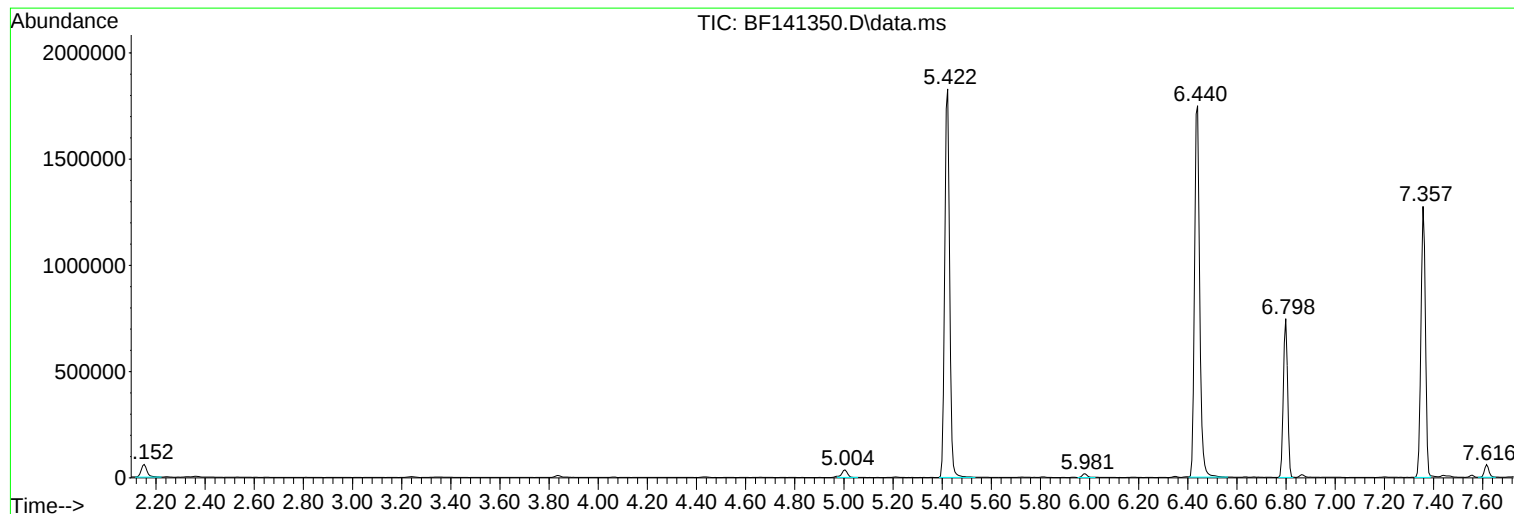
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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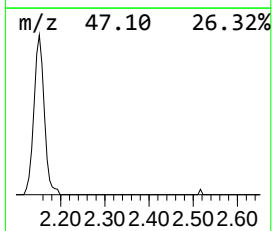
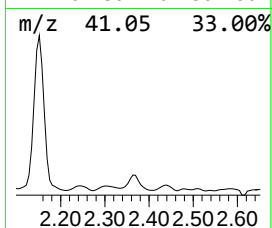
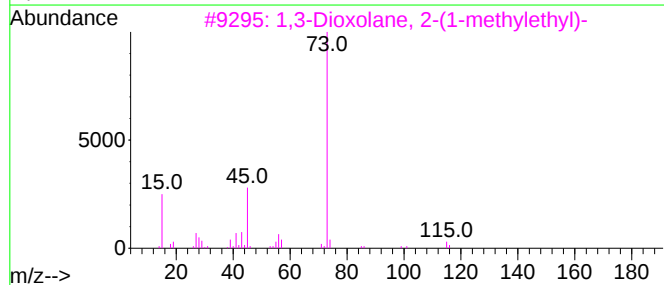
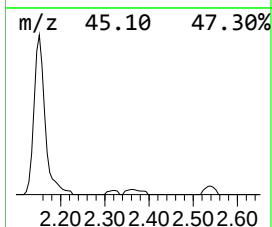
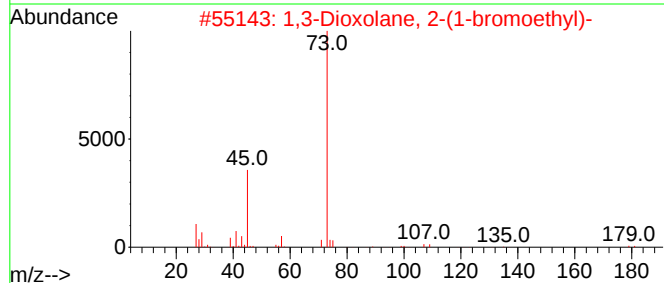
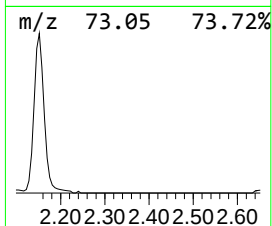
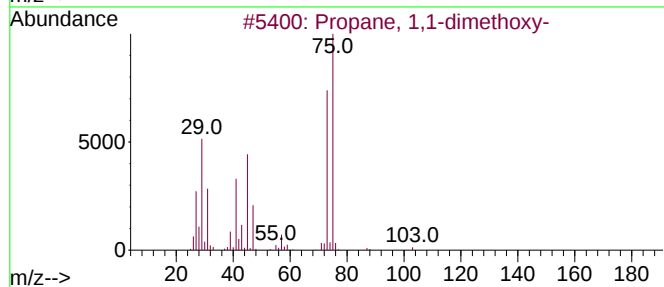
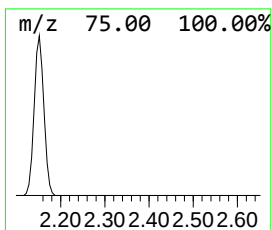
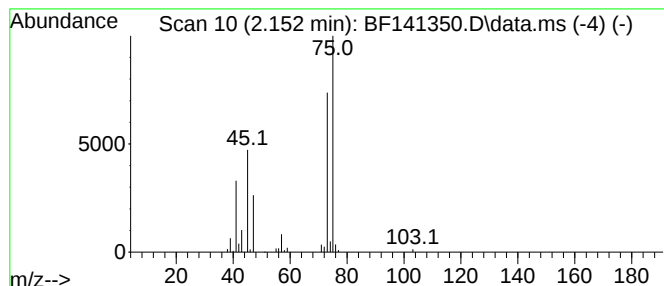
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	2.14 ng	97211	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	27
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
5			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10



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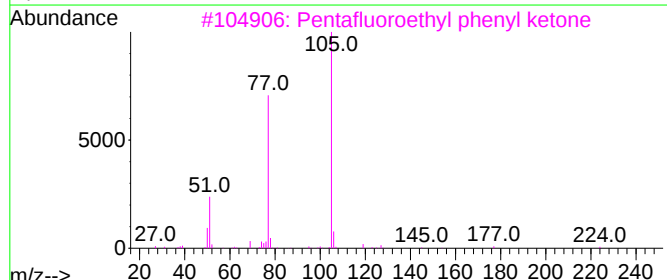
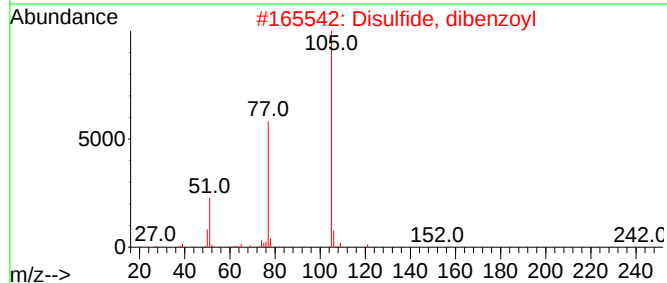
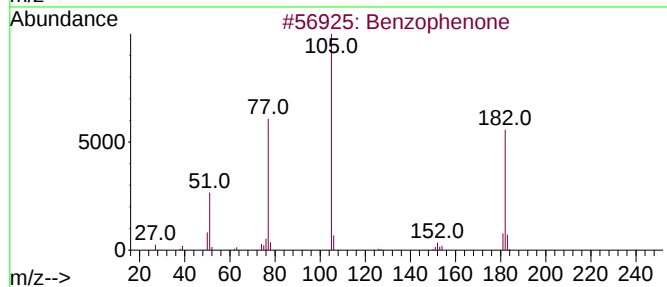
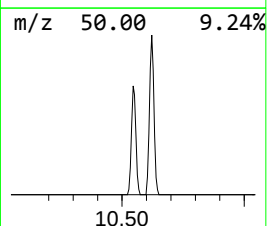
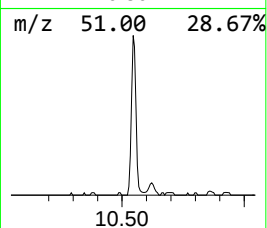
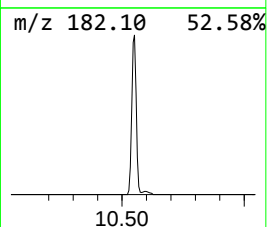
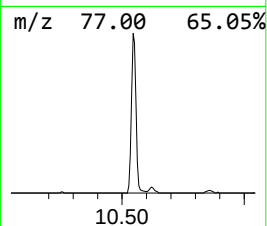
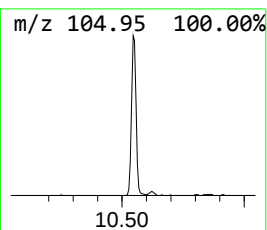
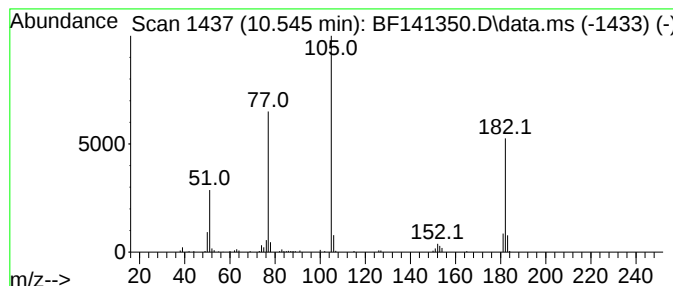
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	2.46 ng	161615	Acenaphthene-d10	9.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52
3			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50



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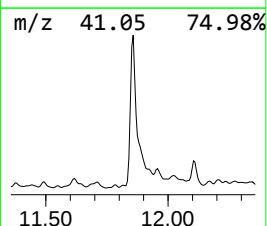
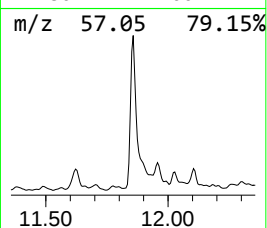
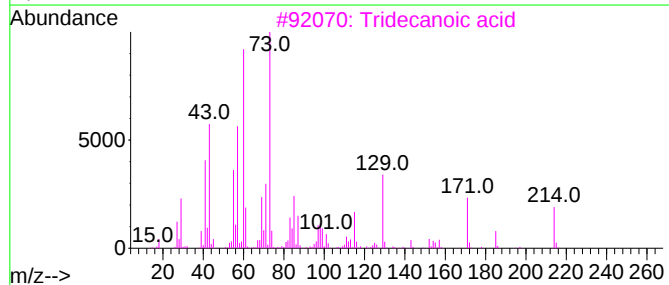
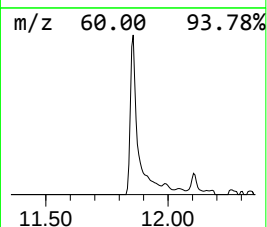
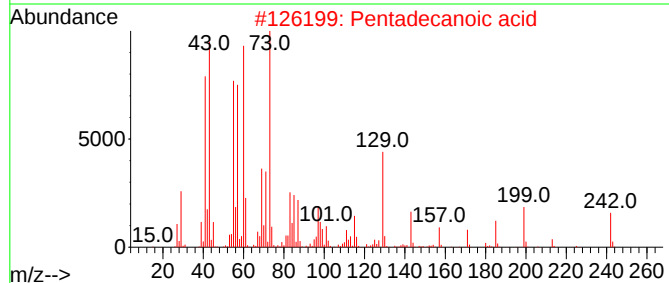
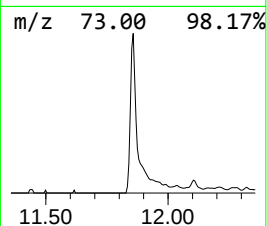
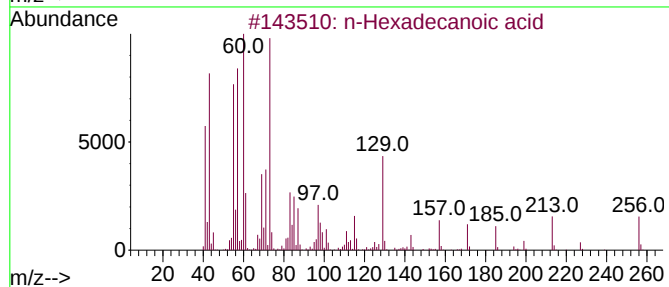
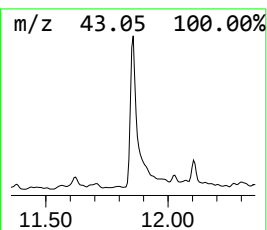
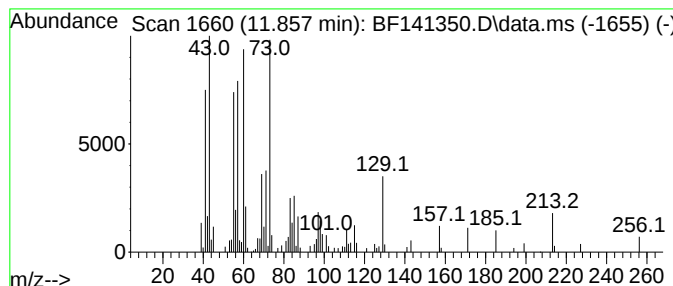
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.91 ng	216106	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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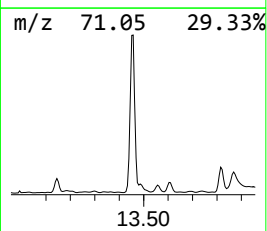
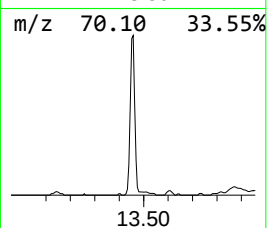
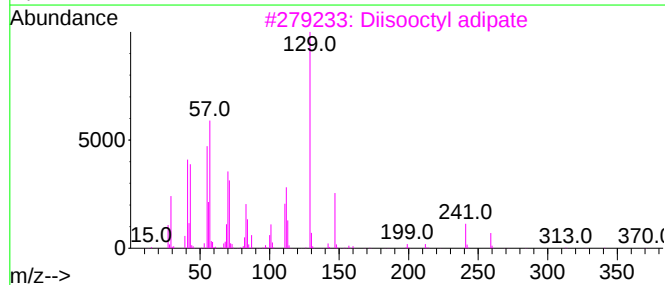
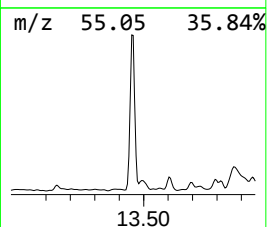
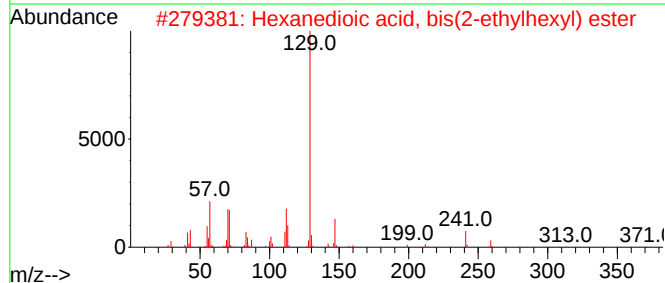
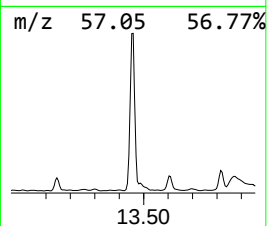
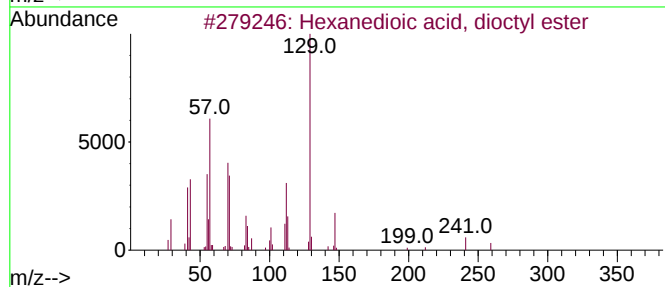
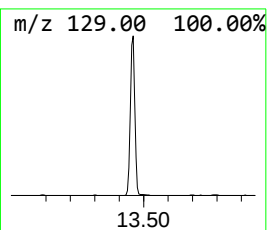
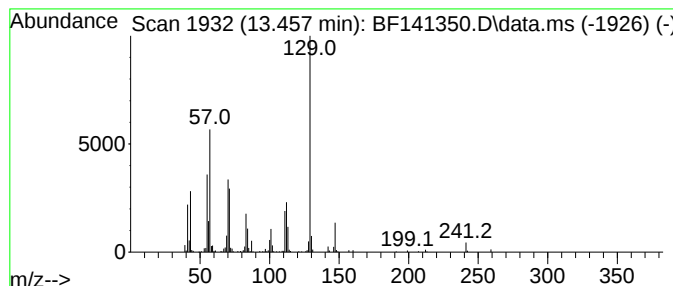
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Peak Number 4 Hexanedioic acid, dioctyl e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	8.52 ng	371571	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
3			Diisooctyl adipate	370	C22H42O4	001330-86-5	86
4			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	80
5			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68



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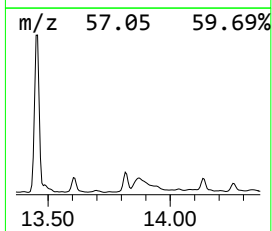
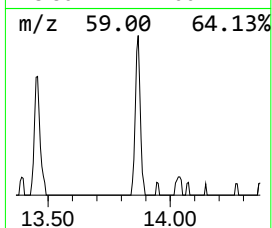
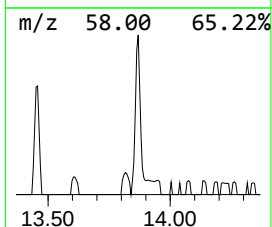
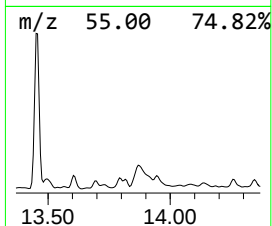
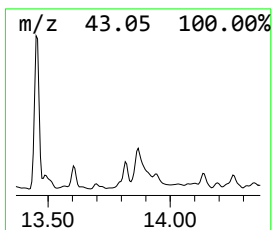
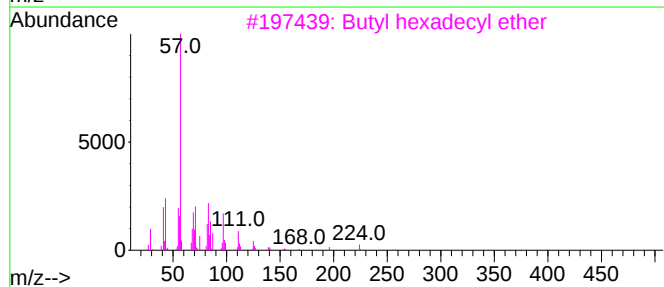
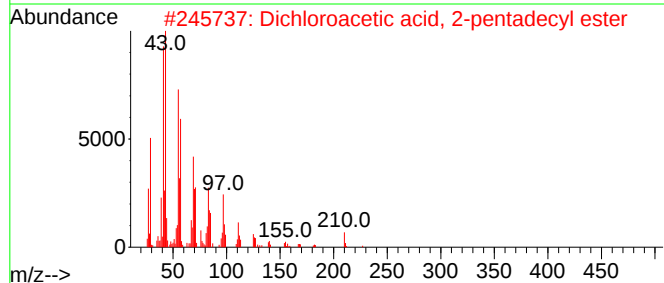
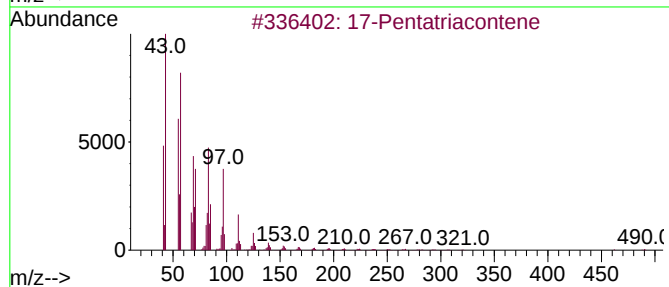
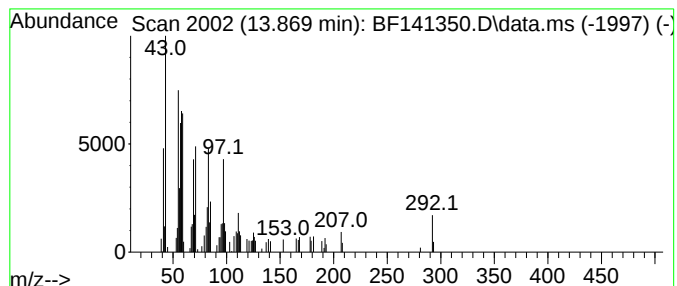
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Peak Number 5 unknown13.869 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	2.21 ng	96260	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	46
2			Dichloroacetic acid, 2-pentadecy...	338	C17H32Cl2O2	1010280-64-7	46
3			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	46
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	42
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013125\
Data File : BF141350.D
Acq On : 31 Jan 2025 23:37
Operator : RC/JU
Sample : Q1194-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

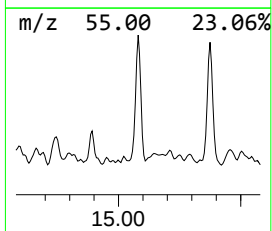
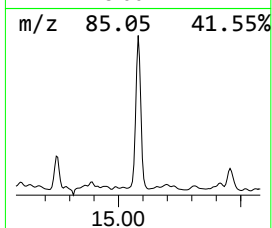
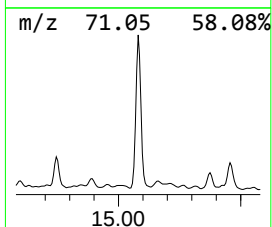
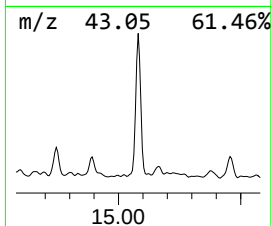
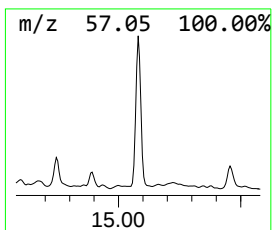
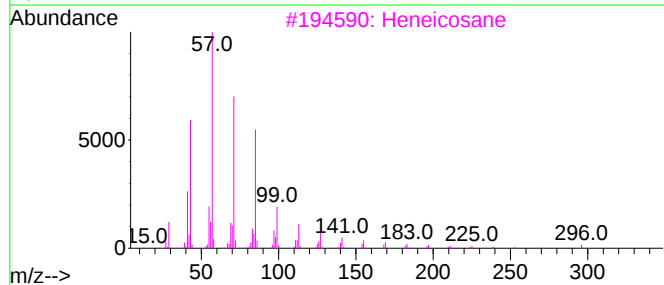
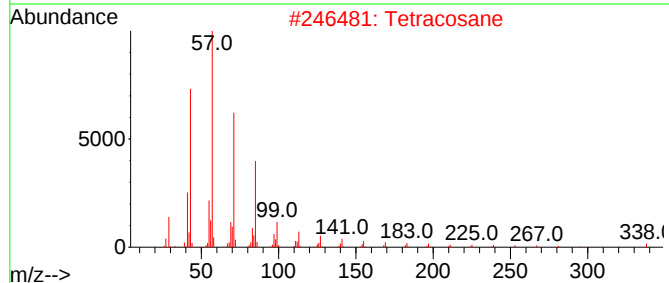
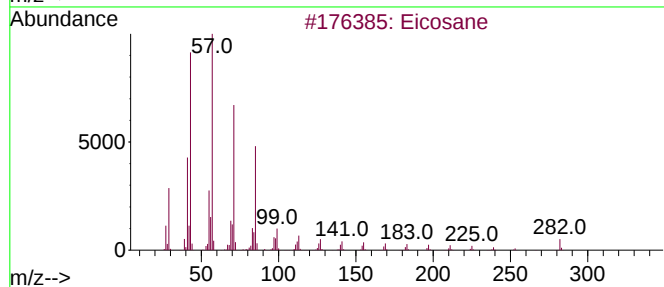
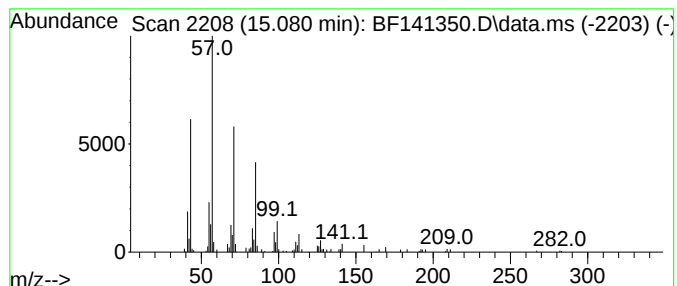
Instrument :
BNA_F
ClientSampleId :
B-110-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.080	2.34 ng	89710	Perylene-d12	15.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013125\
Data File : BF141350.D
Acq On : 31 Jan 2025 23:37
Operator : RC/JU
Sample : Q1194-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-110-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.152	2.1	ng	97211	1	6.798	910293	20.0
Benzophenone	10.545	2.5	ng	161615	3	9.834	1315880	20.0
n-Hexadecanoic ...	11.857	3.9	ng	216106	4	11.322	1105620	20.0
Hexanedioic aci...	13.457	8.5	ng	371571	5	13.963	872438	20.0
unknown13.869	13.869	2.2	ng	96260	5	13.963	872438	20.0
Eicosane	15.080	2.3	ng	89710	6	15.416	768196	20.0
unknown16.739	16.739	2.4	ng	90729	6	15.416	768196	20.0