

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
 Data File : BF140070.D
 Acq On : 26 Oct 2024 20:05
 Operator : RC/JU
 Sample : P4508-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF101824.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140070.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	508	514	521	rBV2	22412	36322	1.14%	0.165%
2	5.504	574	580	585	rBV	1916749	2582591	81.35%	11.727%
3	5.628	596	601	609	rVB	31474	49395	1.56%	0.224%
4	5.992	658	663	670	rBV2	99065	152005	4.79%	0.690%
5	6.122	677	685	694	rVB3	23326	51311	1.62%	0.233%
6	6.269	706	710	711	rBV	47106	59868	1.89%	0.272%
7	6.287	711	713	718	rVB	65444	75298	2.37%	0.342%
8	6.504	744	750	770	rVB	1894874	2709728	85.35%	12.304%
9	6.887	810	815	820	rBV	729290	892455	28.11%	4.052%
10	7.445	903	910	915	rBV	1341786	1793766	56.50%	8.145%
11	7.698	948	953	958	rBV	74973	93108	2.93%	0.423%
12	8.169	1027	1033	1038	rBV	945019	1194647	37.63%	5.424%
13	9.245	1209	1216	1226	rBV	2387200	3174682	100.00%	14.415%
14	9.922	1323	1331	1348	rVV	1038154	1338258	42.15%	6.077%
15	10.351	1397	1404	1408	rBV2	23486	33192	1.05%	0.151%
16	10.633	1447	1452	1459	rBV	229245	286153	9.01%	1.299%
17	10.710	1459	1465	1479	rVV	1265257	1661062	52.32%	7.542%
18	10.827	1480	1485	1493	rVB	29088	50846	1.60%	0.231%
19	11.274	1556	1561	1564	rBV2	21888	31885	1.00%	0.145%
20	11.410	1578	1584	1589	rBV	940622	1185816	37.35%	5.384%
21	11.857	1655	1660	1666	rBV2	26685	49900	1.57%	0.227%
22	11.933	1668	1673	1684	rVV	350439	524232	16.51%	2.380%
23	12.716	1802	1806	1813	rBV	44208	75686	2.38%	0.344%
24	12.992	1848	1853	1861	rVB	1623660	2075917	65.39%	9.426%
25	13.892	2002	2006	2018	rBV2	67438	153386	4.83%	0.696%
26	14.045	2027	2032	2039	rBV	529381	694946	21.89%	3.155%
27	14.804	2158	2161	2167	rBV2	50756	90257	2.84%	0.410%
28	14.904	2174	2178	2184	rVB	136660	190073	5.99%	0.863%
29	15.527	2278	2284	2296	rVB	441040	716705	22.58%	3.254%

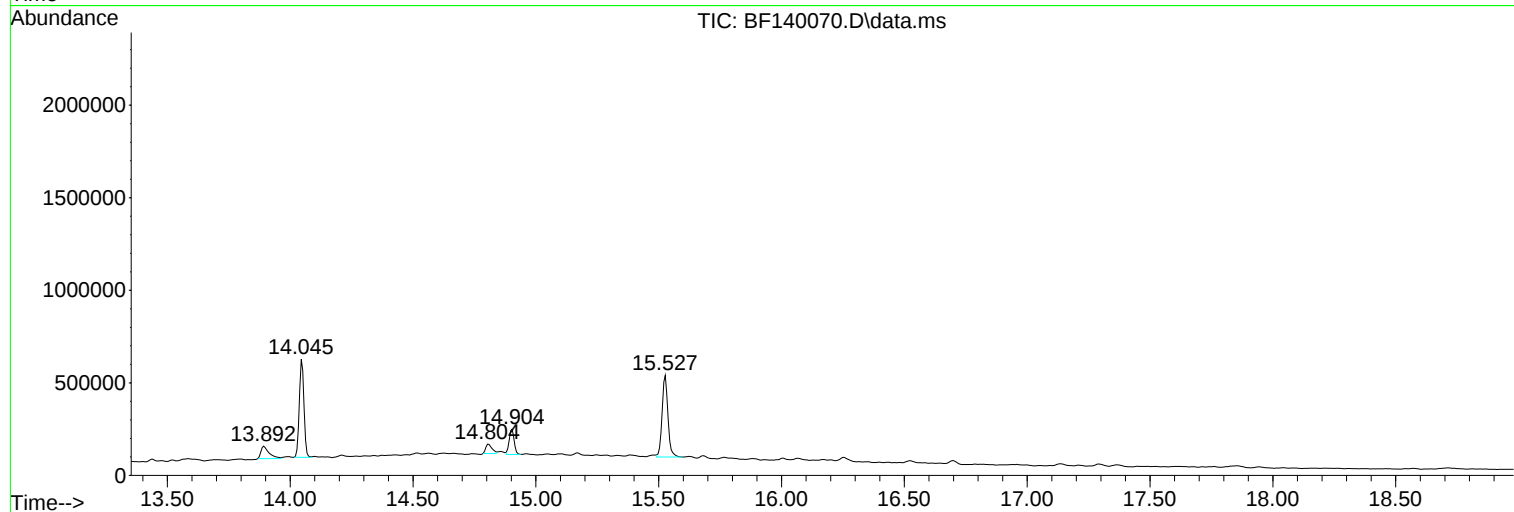
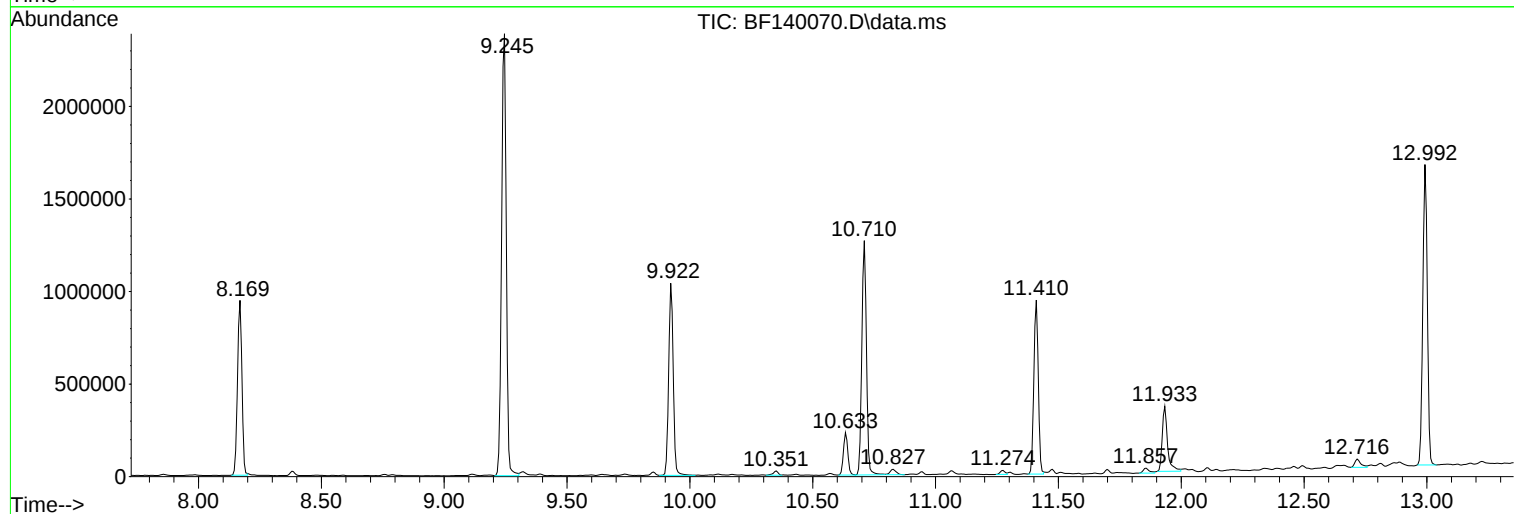
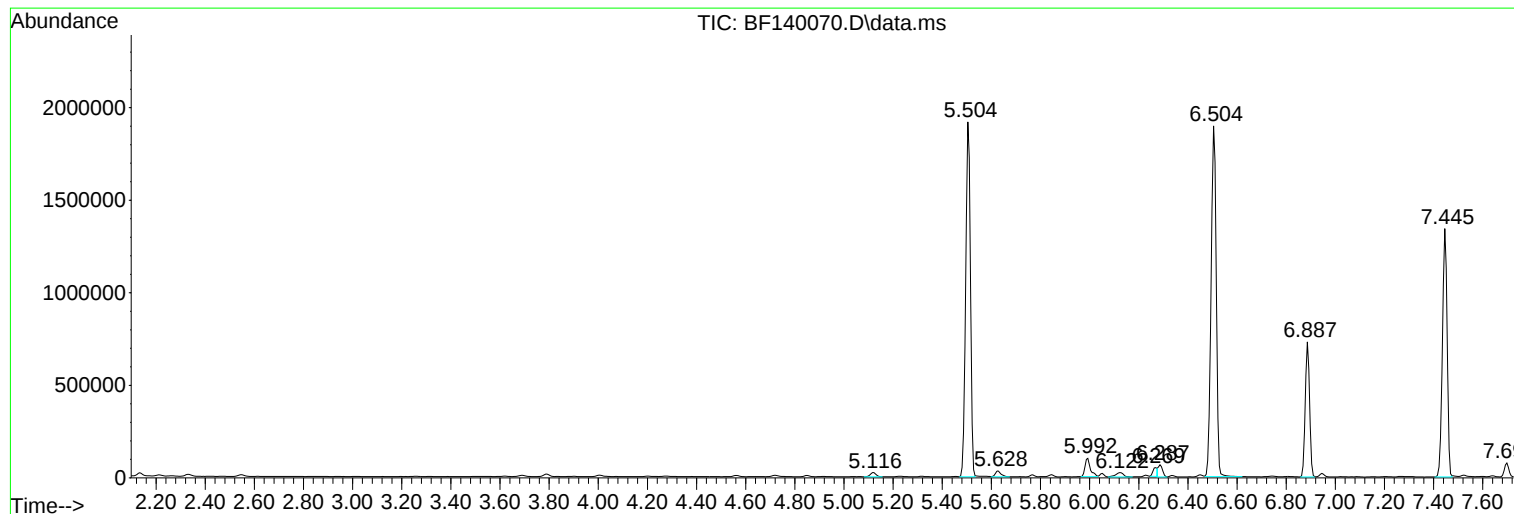
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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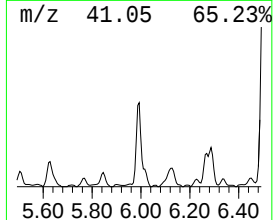
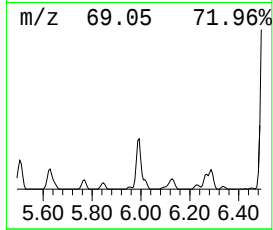
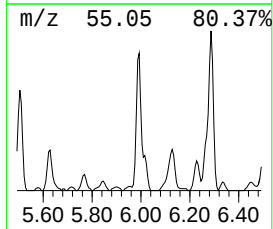
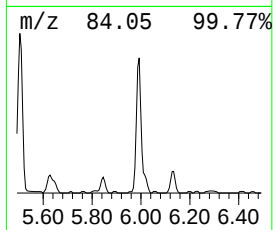
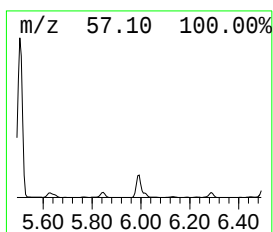
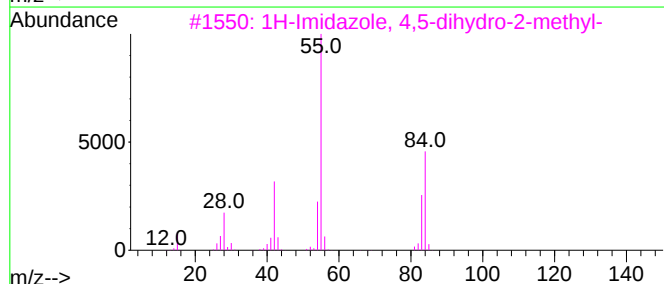
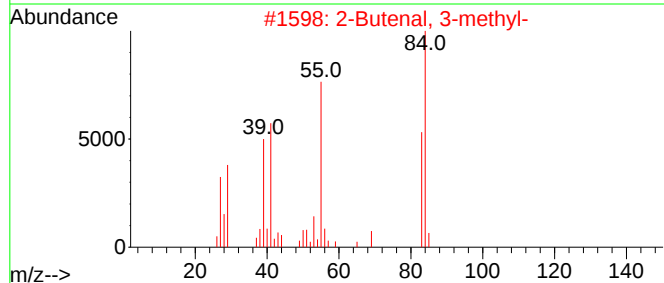
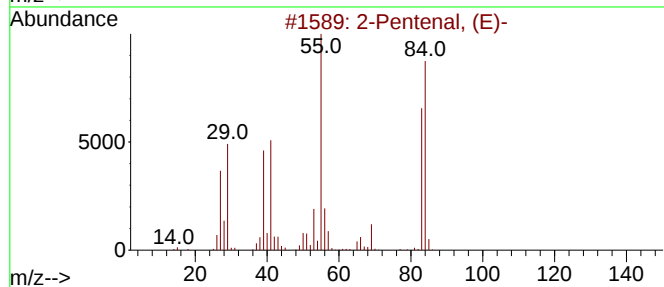
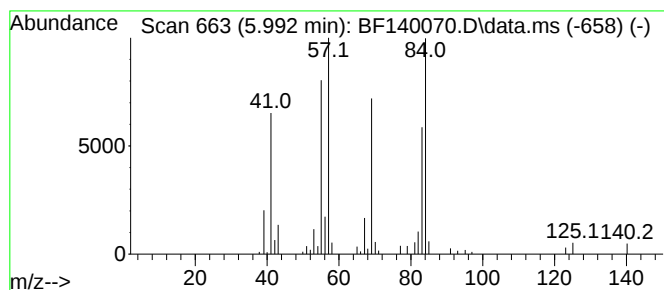
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.992	3.41 ng	152005	1,4-Dichlorobenzene-d4	6.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentenal, (E)-	84	C5H8O	001576-87-0	59
2		2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	53
3		1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	50
4		2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	50
5		Cyclopentanone, 2-(1-methylpropyl)-	140	C9H16O	006376-92-7	47



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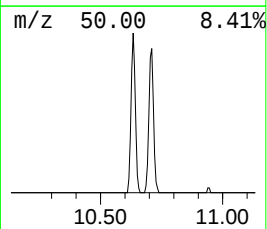
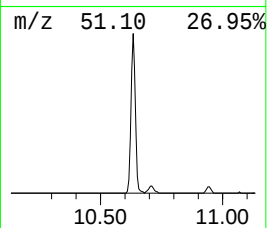
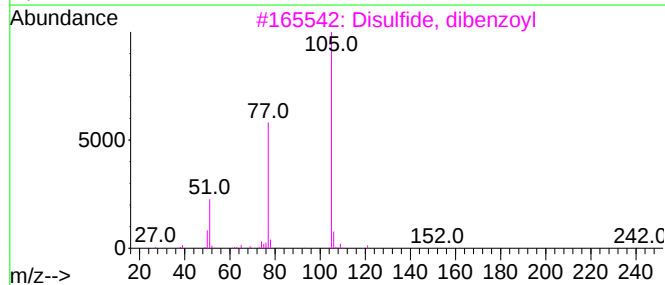
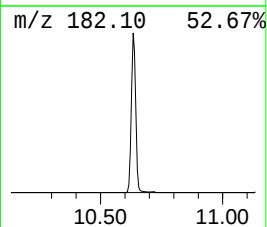
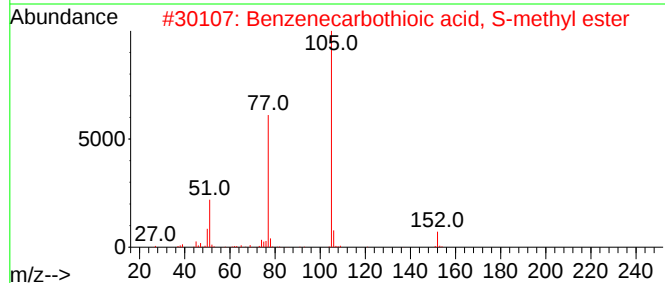
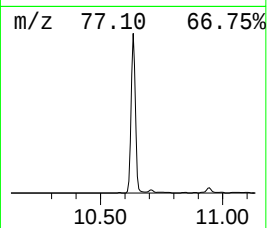
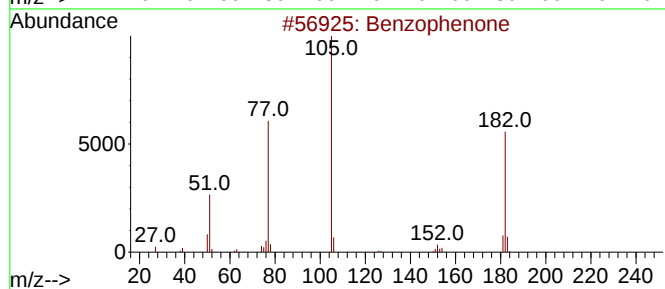
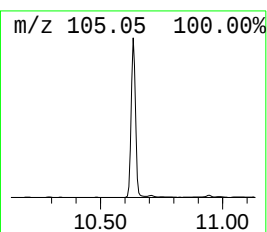
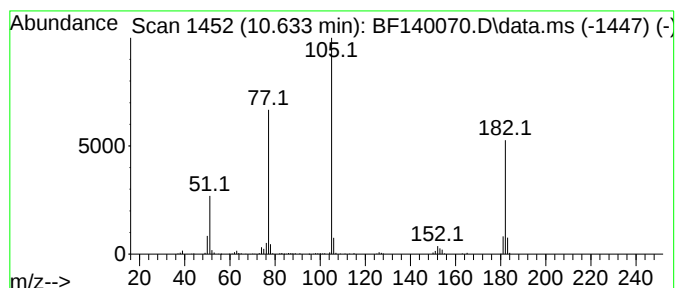
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	4.28 ng	286153	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
3		Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
4		2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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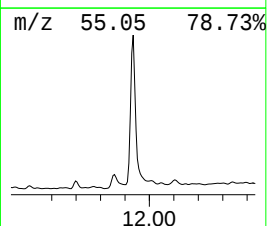
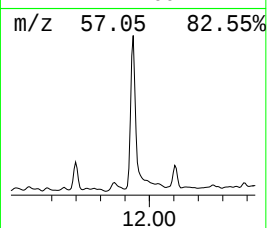
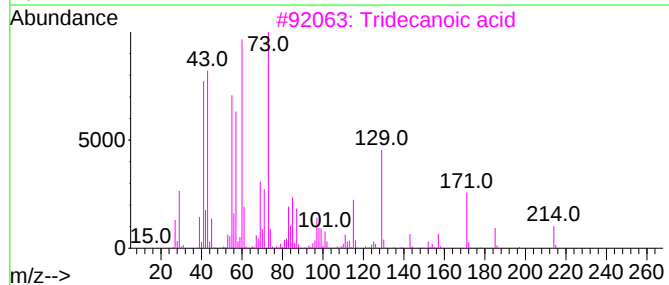
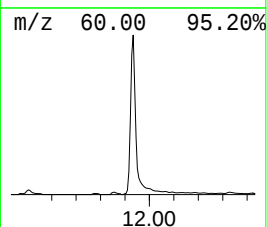
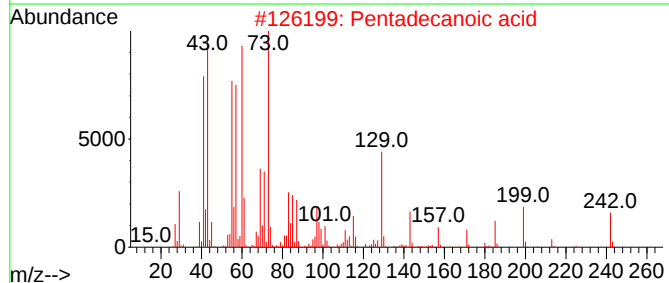
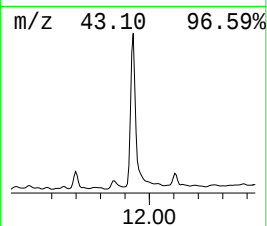
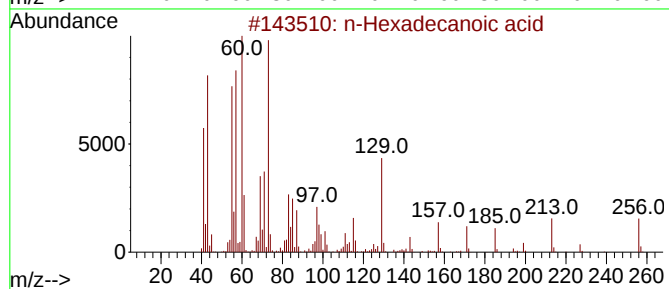
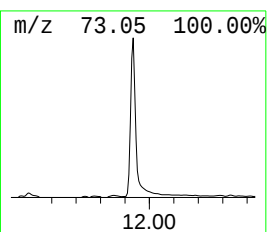
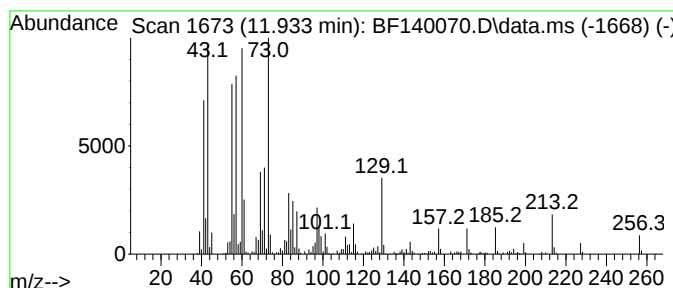
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	8.84 ng	524232	Phenanthrene-d10	11.410	
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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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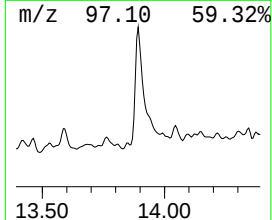
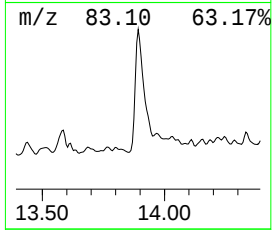
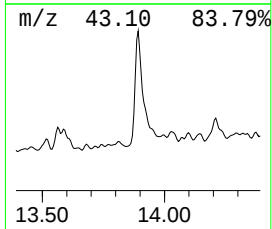
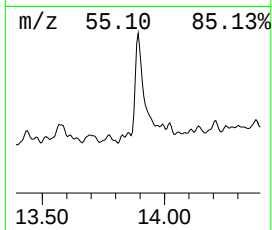
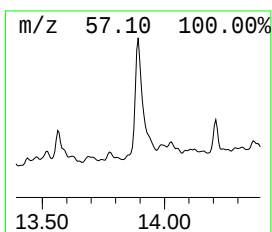
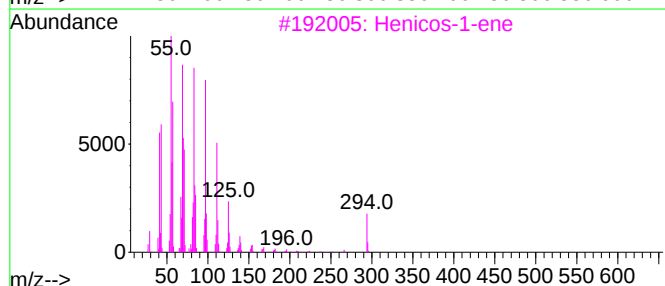
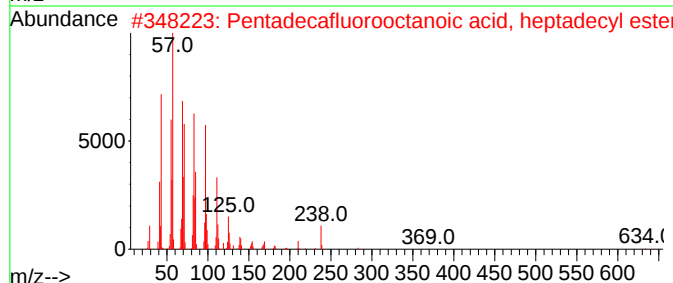
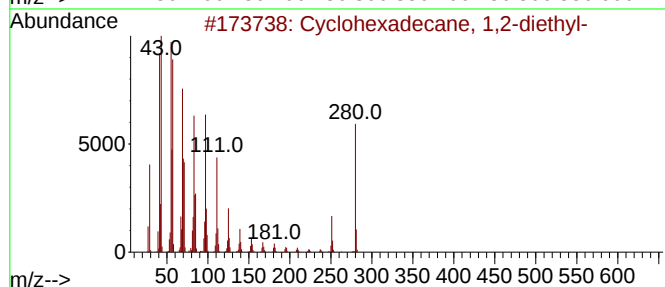
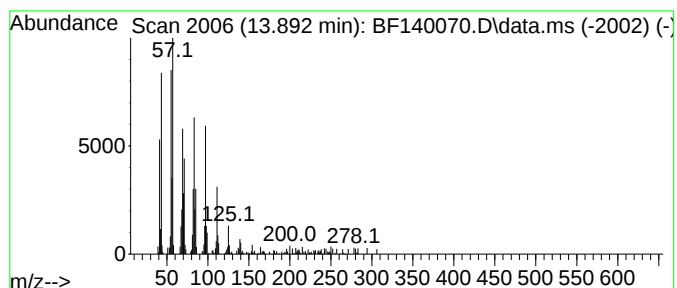
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Peak Number 4 Cyclohexadecane, 1,2-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.41 ng	153386	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	96
2			Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	94
3			Henicos-1-ene	294	C21H42	001599-68-4	93
4			10-Heneicosene (c,t)	294	C21H42	095008-11-0	93
5			1-Hexadecanol	242	C16H34O	036653-82-4	93



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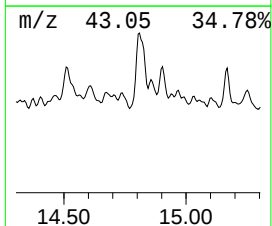
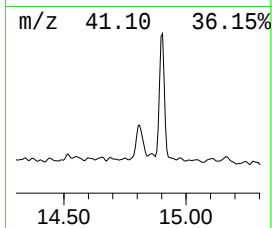
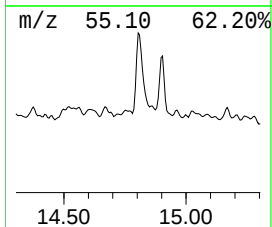
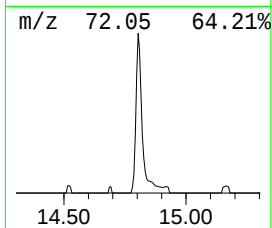
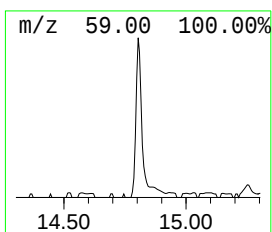
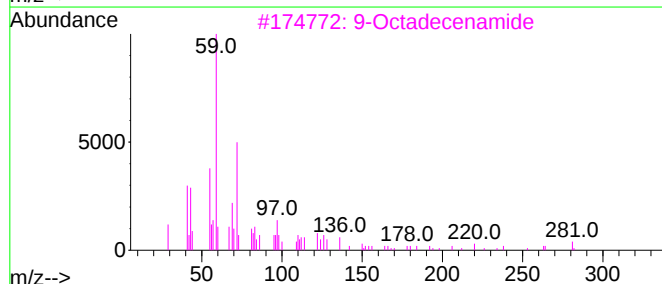
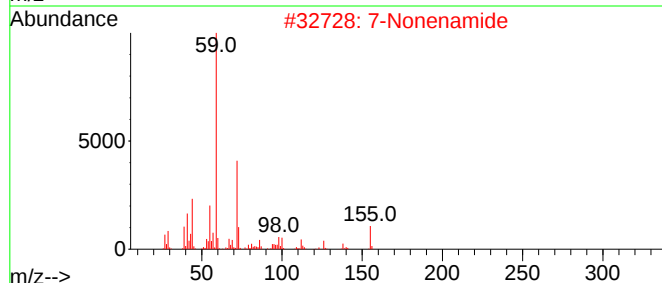
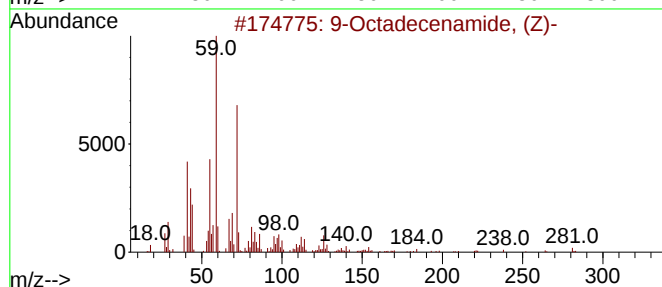
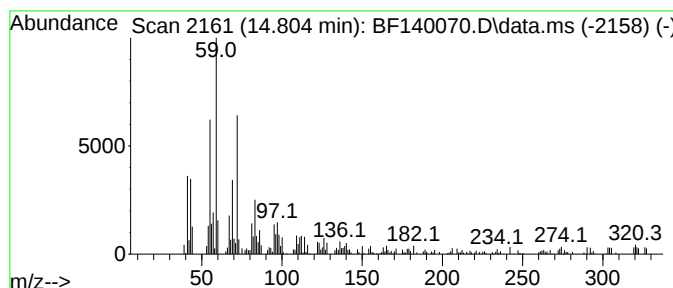
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.52 ng	90257	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			7-Nonenamide	155	C9H17NO	090949-53-4	64
3			9-Octadecenamide	281	C18H35NO	003322-62-1	58
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	58
5			Palmitoleamide	253	C16H31NO	106010-22-4	53



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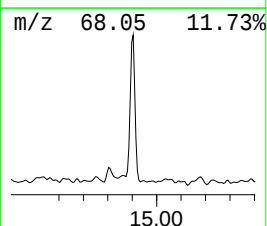
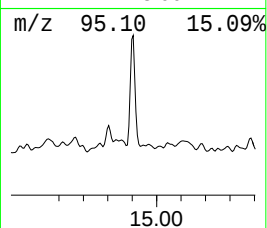
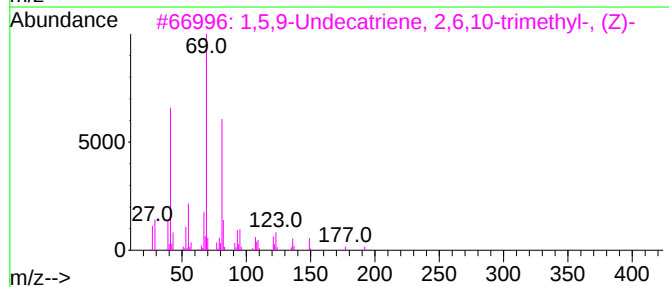
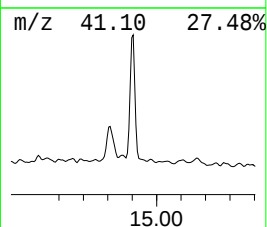
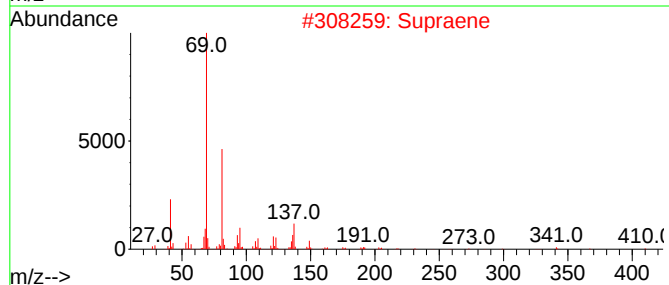
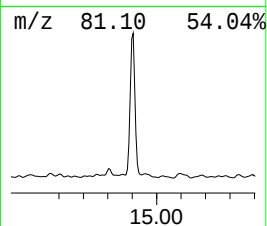
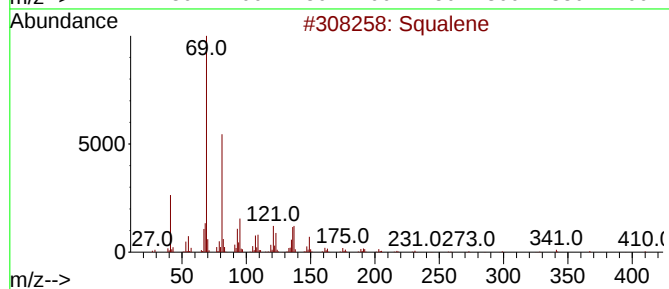
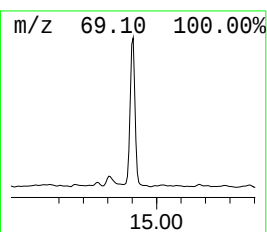
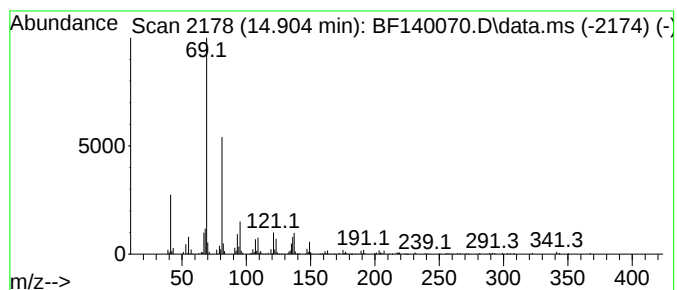
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	5.30 ng	190073	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	87
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			3,7,11-Tridecatricienoic acid, 4,8...	264	C17H28O2	036237-69-1	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140070.D
Acq On : 26 Oct 2024 20:05
Operator : RC/JU
Sample : P4508-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentenal, (E)-	5.992	3.4	ng	152005	1	6.886	892455	20.0
Benzophenone	10.633	4.3	ng	286153	3	9.922	1338260	20.0
n-Hexadecanoic ...	11.933	8.8	ng	524232	4	11.410	1185820	20.0
Cyclohexadecane...	13.892	4.4	ng	153386	5	14.045	694946	20.0
9-Octadecenamid...	14.804	2.5	ng	90257	6	15.527	716705	20.0
Squalene	14.904	5.3	ng	190073	6	15.527	716705	20.0