

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128536.D
 Acq On : 28 May 2022 04:32
 Operator : CG\JU
 Sample : N2954-10
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P044-SS005-0006-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	470	473	480	rVB	85386	100931	2.04%	0.286%
2	5.457	533	539	542	rBV	4197928	4223012	85.49%	11.987%
3	6.292	671	681	691	rBV2	172439	325798	6.60%	0.925%
4	6.463	704	710	713	rBV	3868100	4261727	86.28%	12.096%
5	6.575	725	729	738	rBV	118663	162224	3.28%	0.460%
6	6.840	770	774	777	rBV	1642709	1407675	28.50%	3.996%
7	7.398	864	869	872	rBV	2917723	2892231	58.55%	8.209%
8	7.863	945	948	953	rVB	59572	52599	1.06%	0.149%
9	8.122	987	992	995	rBV	2077950	1823269	36.91%	5.175%
10	9.198	1169	1175	1178	rBV	5422231	4939695	100.00%	14.021%
11	9.875	1284	1290	1294	rBV	2302178	1927949	39.03%	5.472%
12	10.663	1418	1424	1427	rBV	3122753	2701432	54.69%	7.668%
13	11.363	1539	1543	1546	rBV	2049865	1741809	35.26%	4.944%
14	11.892	1629	1633	1637	rBV	302396	281334	5.70%	0.799%
15	12.674	1763	1766	1774	rBV	114982	144462	2.92%	0.410%
16	12.951	1809	1813	1816	rBV	4060033	3644127	73.77%	10.343%
17	13.892	1964	1973	1985	rBV5	83762	295199	5.98%	0.838%
18	13.998	1987	1991	1995	rBV	1274394	1255856	25.42%	3.565%
19	14.104	2002	2009	2019	rBV	946238	1189530	24.08%	3.376%
20	14.533	2078	2082	2087	rBV7	28295	55665	1.13%	0.158%
21	15.133	2180	2184	2188	rBV	83985	85637	1.73%	0.243%
22	15.215	2192	2198	2206	rBV9	40433	103586	2.10%	0.294%
23	15.468	2235	2241	2246	rBV	1010218	1196502	24.22%	3.396%
24	15.957	2319	2324	2328	rBV	112195	152125	3.08%	0.432%
25	16.756	2457	2460	2468	rVB7	31785	53326	1.08%	0.151%
26	17.062	2508	2512	2520	rVB2	50915	99821	2.02%	0.283%
27	17.604	2597	2604	2615	rVB2	30047	113758	2.30%	0.323%

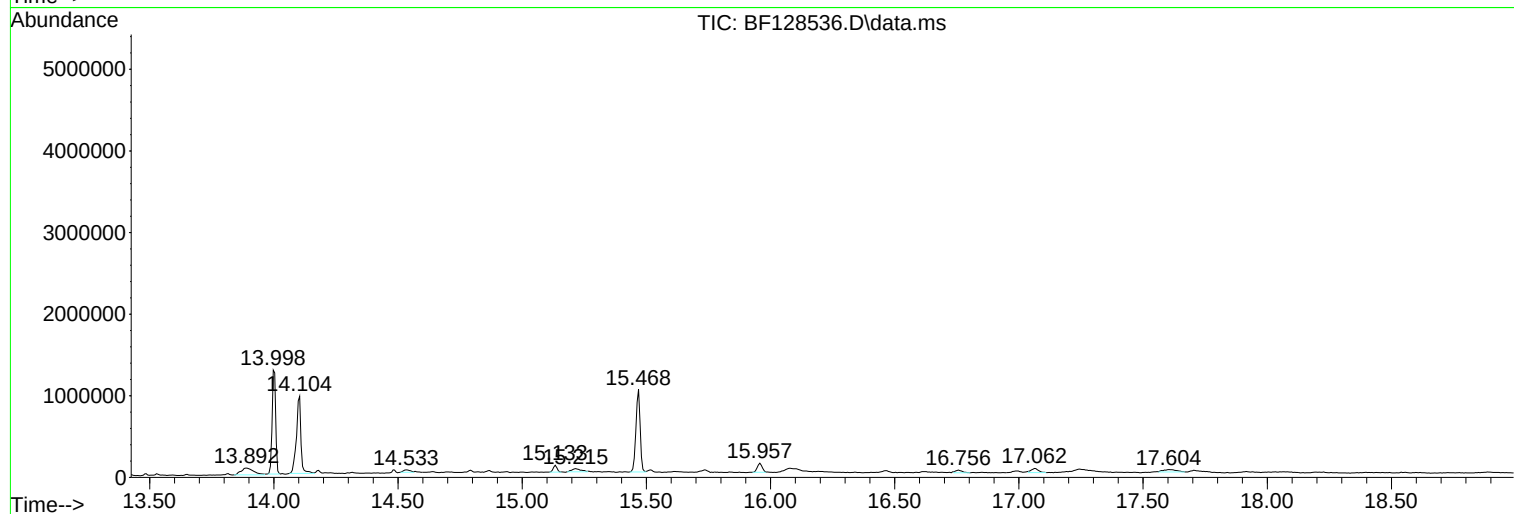
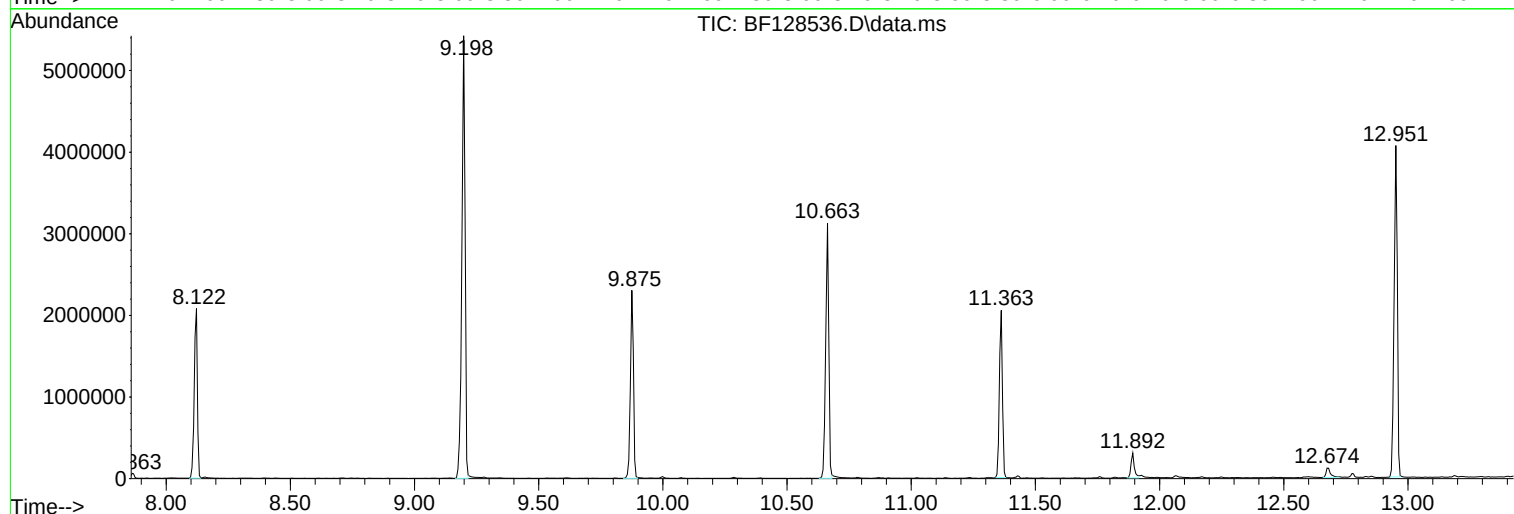
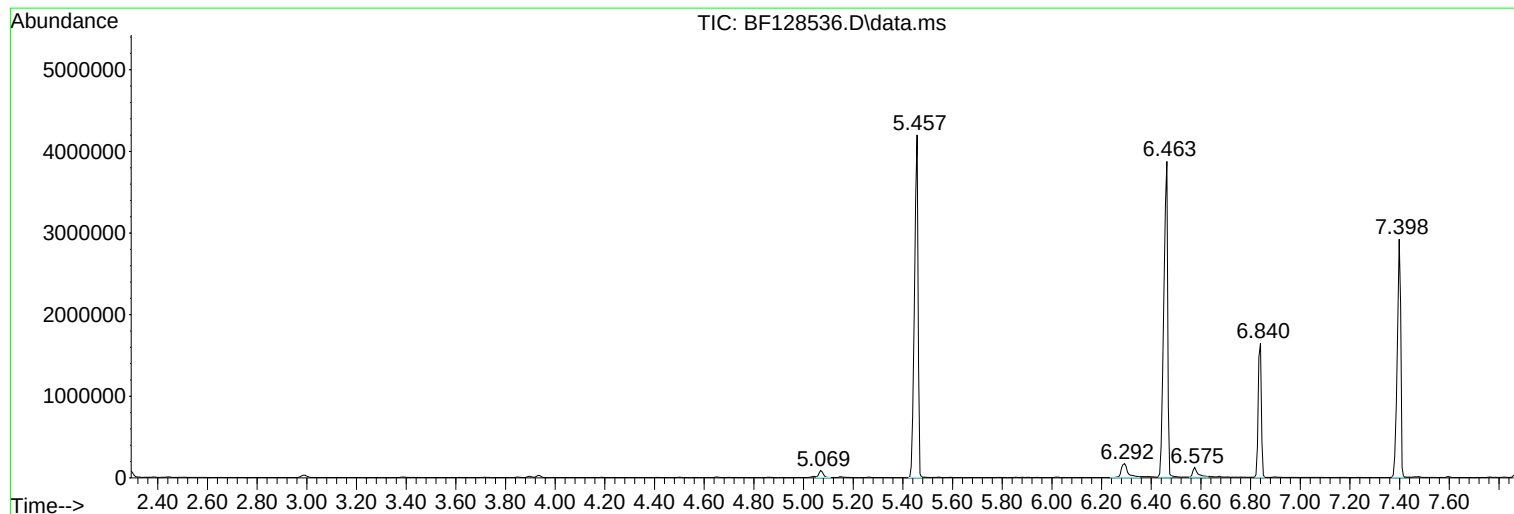
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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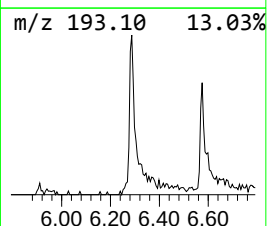
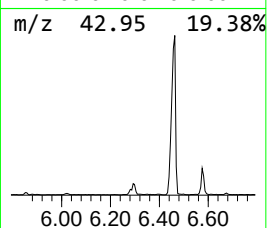
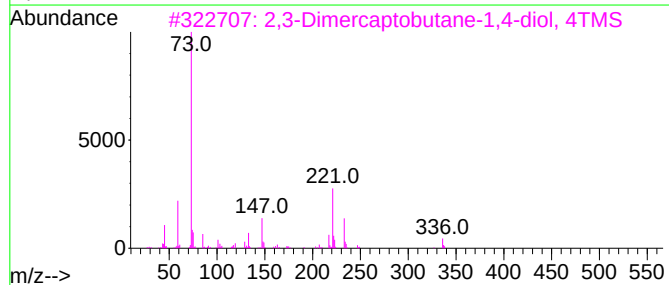
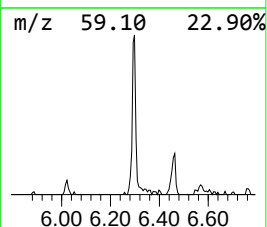
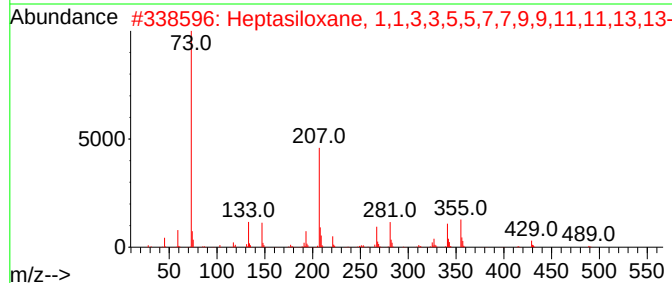
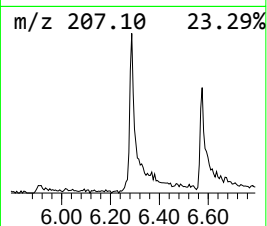
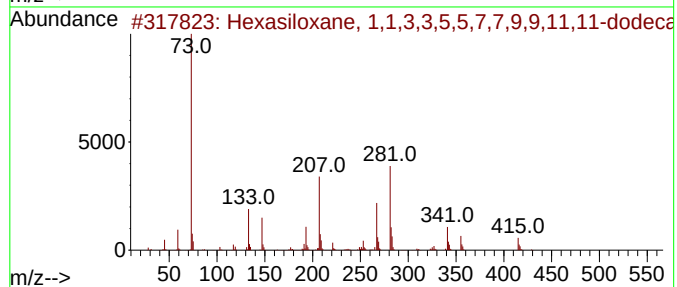
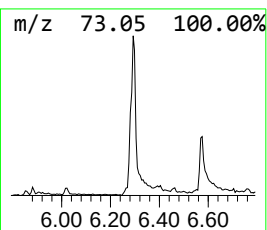
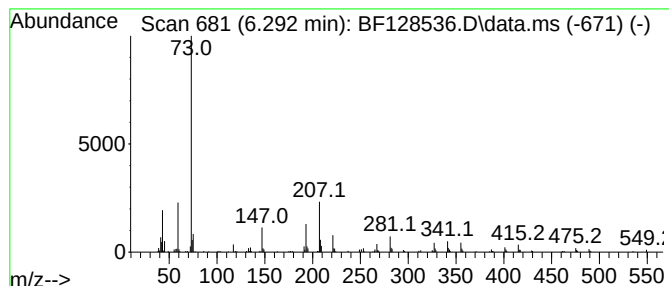
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Peak Number 1 unknown6.292 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.292	4.63 ng	325798	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	38
2			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	38
3			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	32
4			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	22
5			Tetrasiloxane, 3,5-diethoxy-1,1,...	518	C16H46O7Si6	072439-78-2	16



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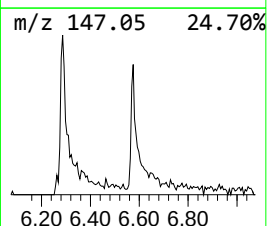
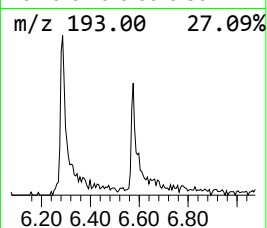
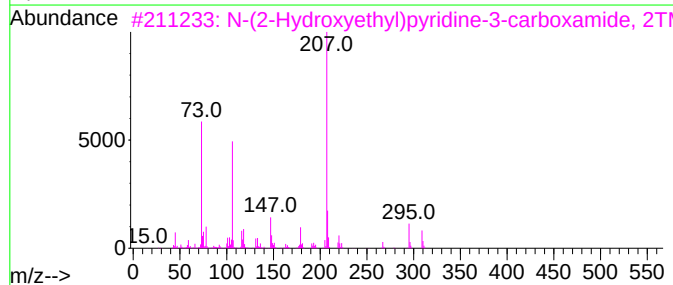
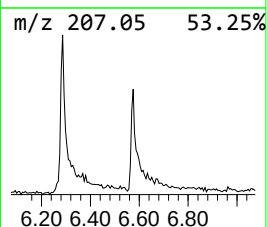
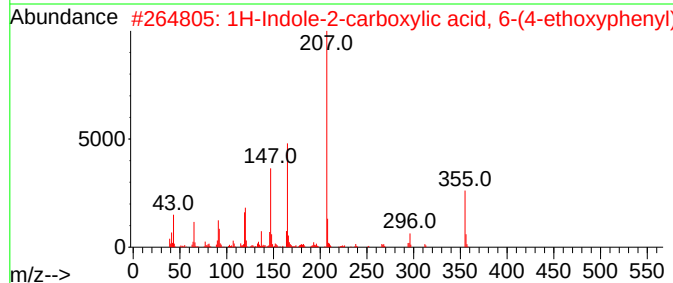
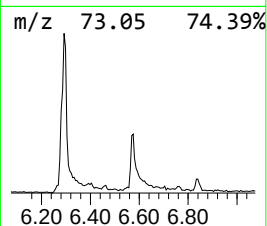
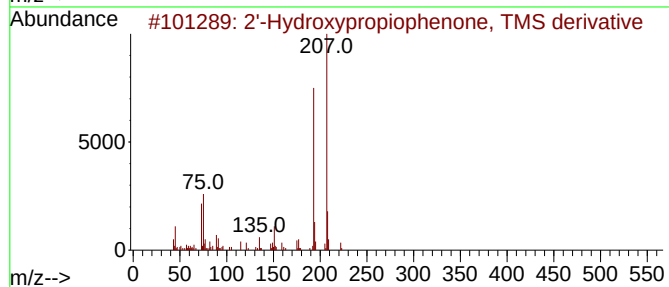
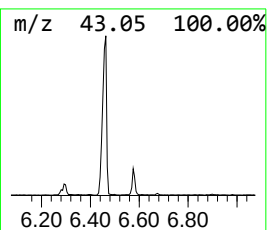
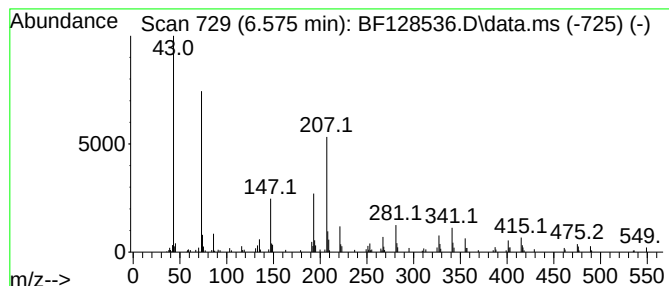
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Peak Number 2 unknown6.575 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.575	2.30 ng	162224	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2'-Hydroxypropiophenone, TMS der...	222	C12H18O2Si	033342-87-9	37
2			1H-Indole-2-carboxylic acid, 6-(...	355	C21H25NO4	1010316-17-5	27
3			N-(2-Hydroxyethyl)pyridine-3-car...	310	C14H26N2O2Si2	1000485-24-9	27
4			8-Methoxy-3-oxo-2,4-dihydro-1,4-...	207	C10H9NO4	711021-34-0	27
5			Benz[b]-1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	27



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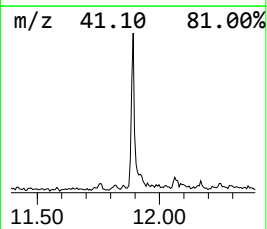
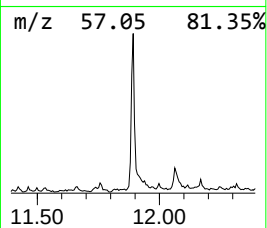
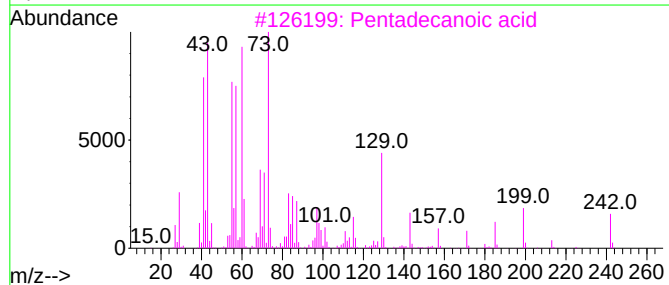
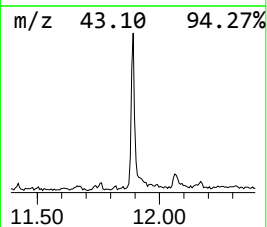
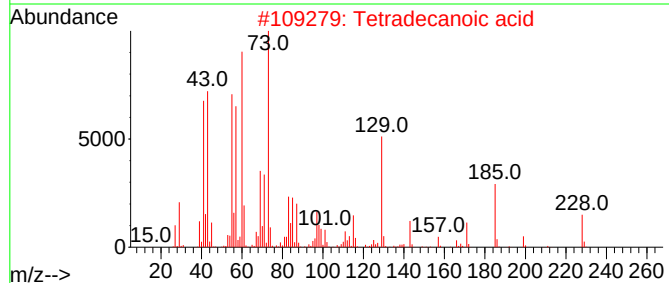
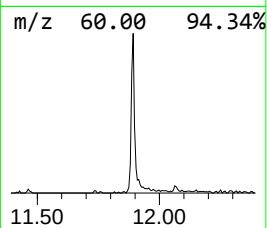
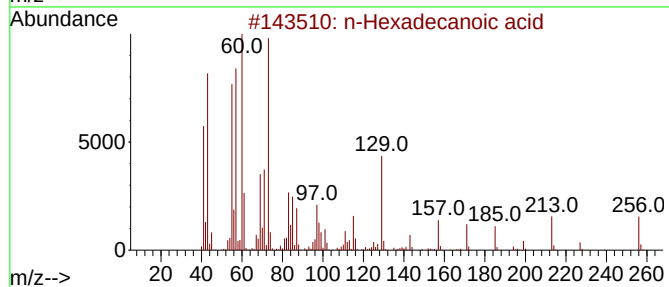
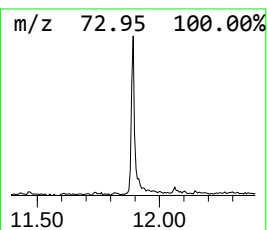
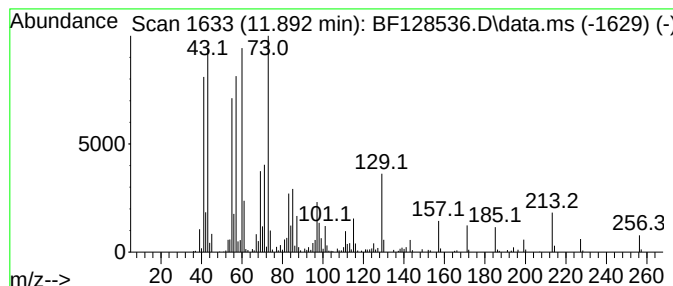
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.23 ng	281334	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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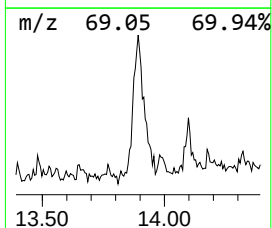
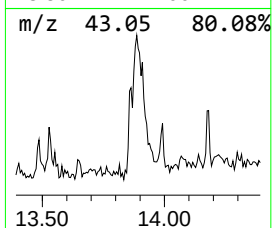
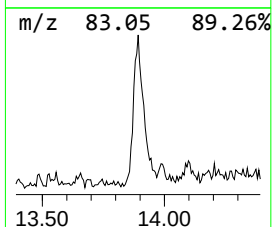
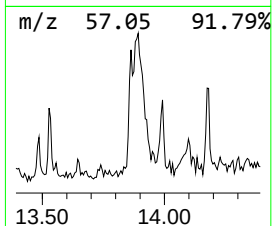
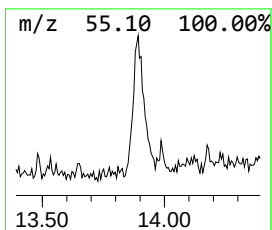
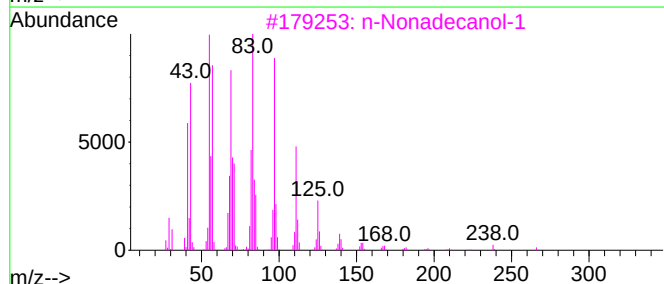
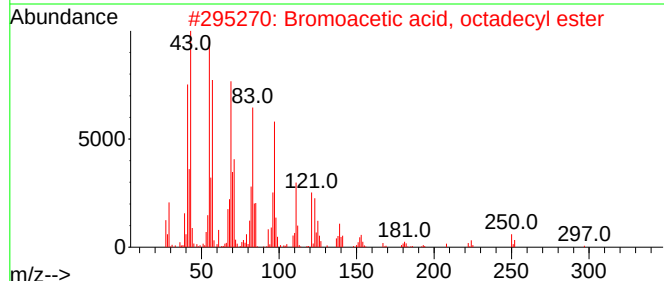
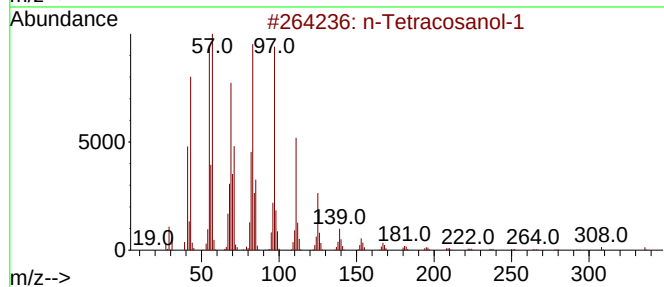
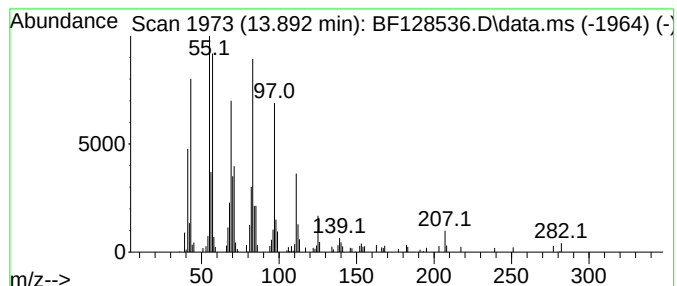
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.70 ng	295199	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4			Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	87
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	81



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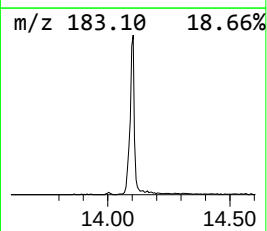
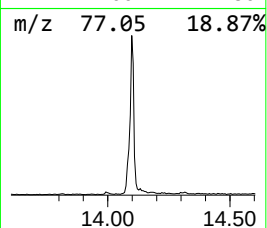
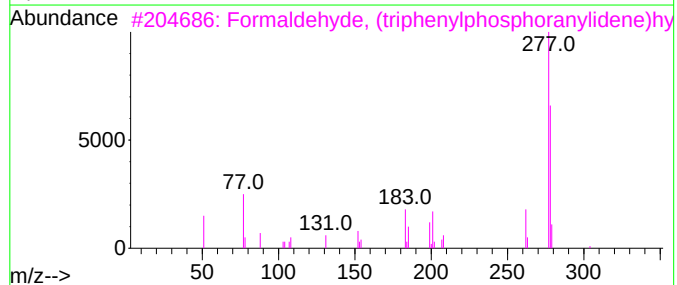
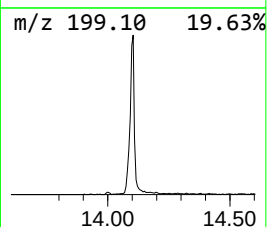
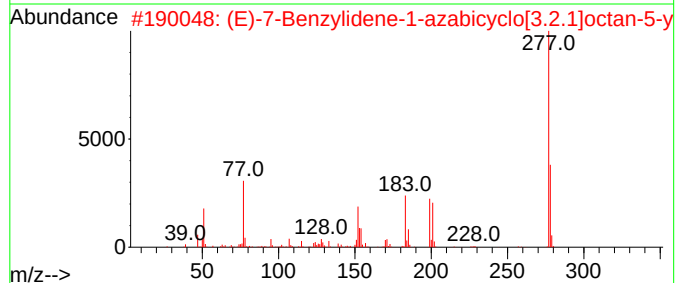
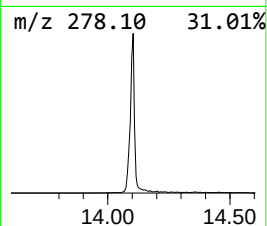
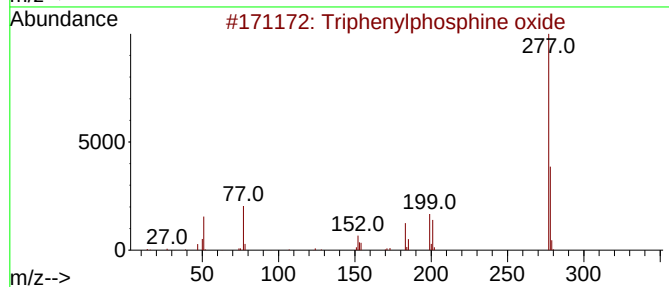
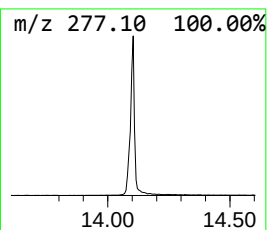
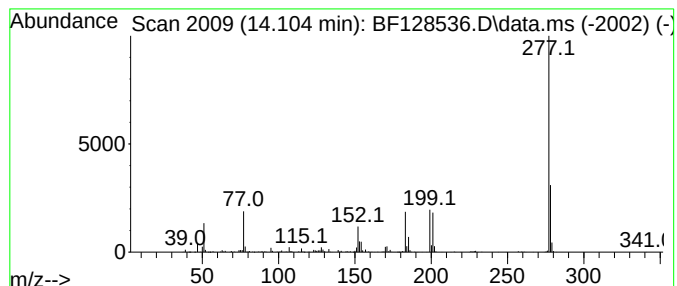
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	18.94 ng	1189530	Chrysene-d12	14.004

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	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



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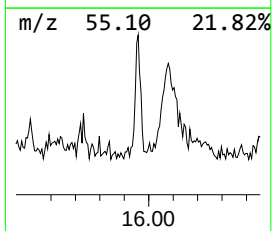
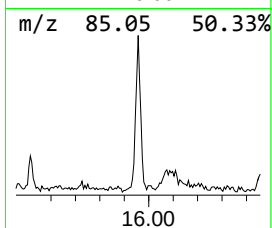
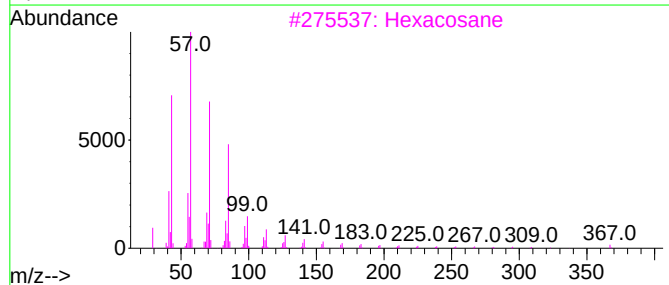
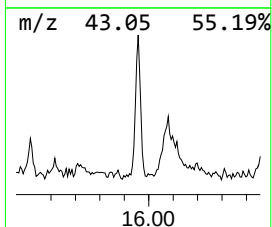
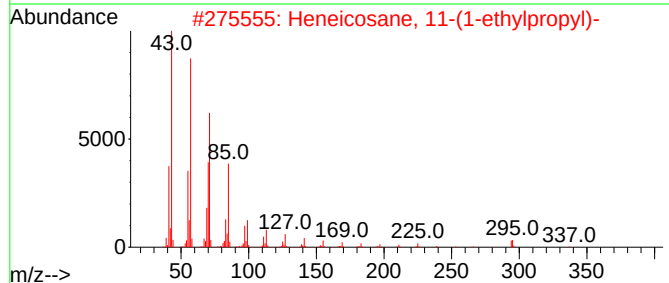
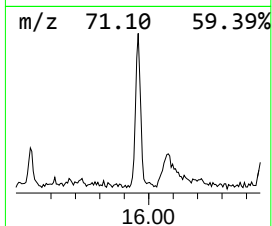
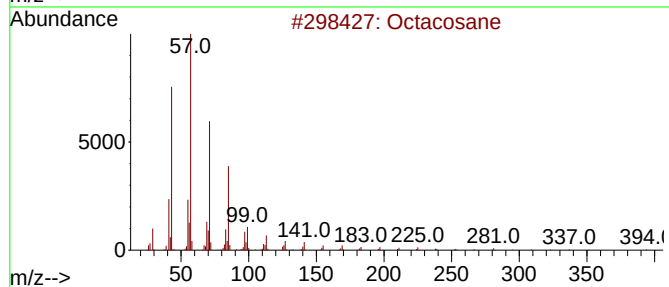
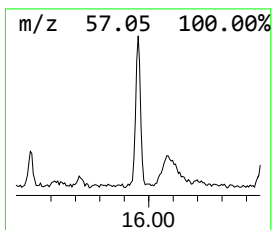
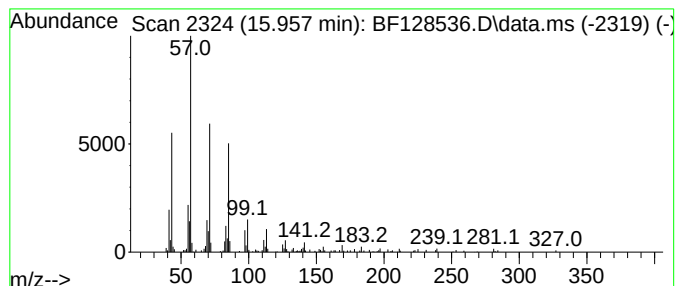
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.54 ng	152125	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128536.D
Acq On : 28 May 2022 04:32
Operator : CG\JU
Sample : N2954-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P044-SS005-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
unknown6.292	6.292	4.6	ng	325798	1	6.840	1407680	20.0
unknown6.575	6.575	2.3	ng	162224	1	6.840	1407680	20.0
n-Hexadecanoic ...	11.892	3.2	ng	281334	4	11.363	1741810	20.0
n-Tetracosanol-1	13.892	4.7	ng	295199	5	14.004	1255860	20.0
Triphenylphosph...	14.104	18.9	ng	1189530	5	14.004	1255860	20.0
Octacosane	15.957	2.5	ng	152125	6	15.468	1196500	20.0