

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021225\
 Data File : BF141599.D
 Acq On : 12 Feb 2025 19:12
 Operator : RC/JU
 Sample : Q1343-05
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-10

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	558	563	582	rBV	1197412	1631068	87.89%	10.852%
2	6.422	731	736	758	rBV	1203982	1682491	90.66%	11.194%
3	6.786	792	798	807	rBV	433822	618046	33.30%	4.112%
4	7.345	887	893	905	rBV	796029	1079710	58.18%	7.184%
5	7.610	933	938	954	rBV	30165	59467	3.20%	0.396%
6	8.069	1010	1016	1035	rBV	469034	649496	35.00%	4.321%
7	8.298	1051	1055	1066	rVB	17764	29291	1.58%	0.195%
8	8.428	1071	1077	1095	rBV2	13144	56277	3.03%	0.374%
9	9.139	1193	1198	1209	rBV	1427154	1855869	100.00%	12.348%
10	9.822	1308	1314	1328	rBV	534407	708628	38.18%	4.715%
11	10.533	1430	1435	1443	rBV	399682	502129	27.06%	3.341%
12	10.610	1443	1448	1465	rVV	865046	1145677	61.73%	7.623%
13	10.845	1482	1488	1495	rBV	57097	80291	4.33%	0.534%
14	11.304	1561	1566	1576	rBV2	539420	797673	42.98%	5.307%
15	11.380	1576	1579	1585	rVB	13835	19002	1.02%	0.126%
16	11.839	1653	1657	1667	rVV2	79186	180481	9.72%	1.201%
17	11.921	1667	1671	1680	rVB	27512	60876	3.28%	0.405%
18	12.086	1695	1699	1705	rBV3	9812	19665	1.06%	0.131%
19	12.327	1735	1740	1743	rBV	25589	35045	1.89%	0.233%
20	12.516	1767	1772	1778	rBV	162901	223389	12.04%	1.486%
21	12.745	1804	1811	1816	rBV2	146455	222534	11.99%	1.481%
22	12.798	1817	1820	1826	rVB3	13024	18872	1.02%	0.126%
23	12.892	1828	1836	1843	rBV	1195647	1554954	83.79%	10.346%
24	12.963	1844	1848	1854	rVB3	13724	25125	1.35%	0.167%
25	13.074	1860	1867	1871	rBV3	16758	35120	1.89%	0.234%
26	13.145	1872	1879	1881	rBV4	10041	20223	1.09%	0.135%
27	13.186	1881	1886	1892	rVB3	24317	51955	2.80%	0.346%
28	13.463	1930	1933	1943	rVB9	7248	18885	1.02%	0.126%
29	13.586	1951	1954	1961	rVB	15246	22734	1.22%	0.151%
30	13.792	1986	1989	1998	rVB2	17697	27054	1.46%	0.180%
31	13.945	2008	2015	2028	rVB2	379654	639850	34.48%	4.257%
32	14.415	2091	2095	2100	rBV4	13169	22626	1.22%	0.151%
33	14.792	2154	2159	2163	rBV	34109	50584	2.73%	0.337%
34	14.974	2185	2190	2199	rBV	68654	154988	8.35%	1.031%
35	15.268	2235	2240	2246	rVB	36478	56687	3.05%	0.377%
36	15.333	2246	2251	2256	rBV	44212	69767	3.76%	0.464%

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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-BF020625.M
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37	15.392	2256	2261	2274	rVB	275099	454073	24.47%	3.021%
38	15.839	2332	2337	2341	rBV	17381	30733	1.66%	0.204%
39	16.092	2376	2380	2387	rVB7	13477	25130	1.35%	0.167%
40	16.827	2499	2505	2514	rVB2	26118	65601	3.53%	0.436%
41	17.262	2574	2579	2585	rVB2	13121	27800	1.50%	0.185%

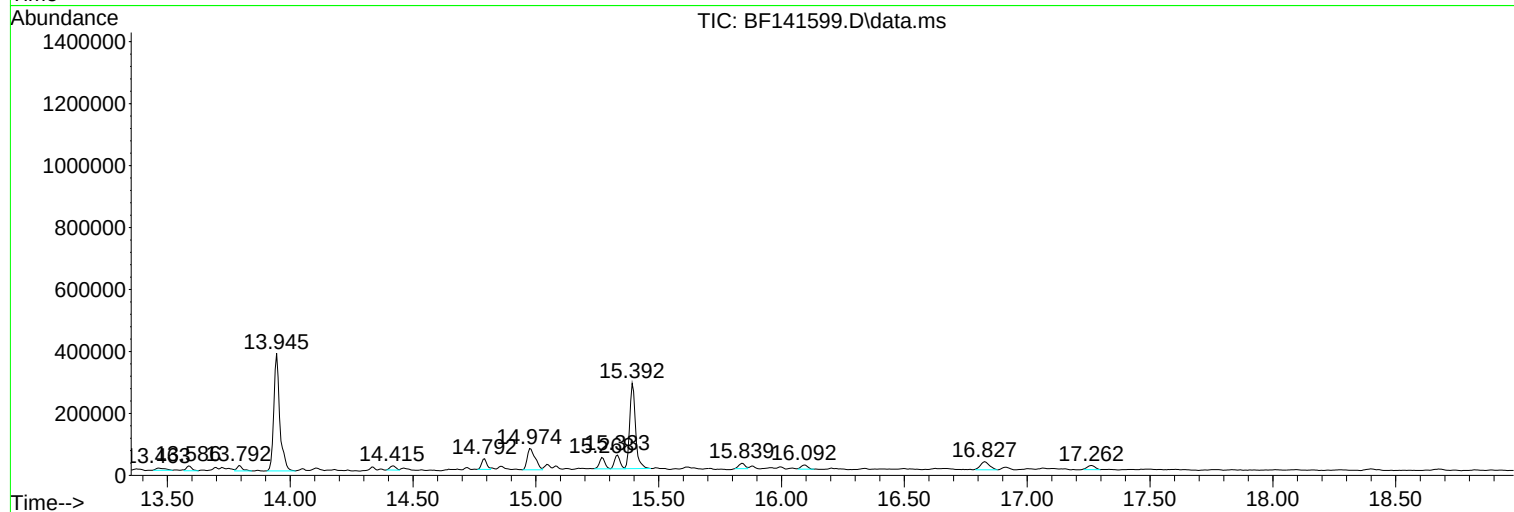
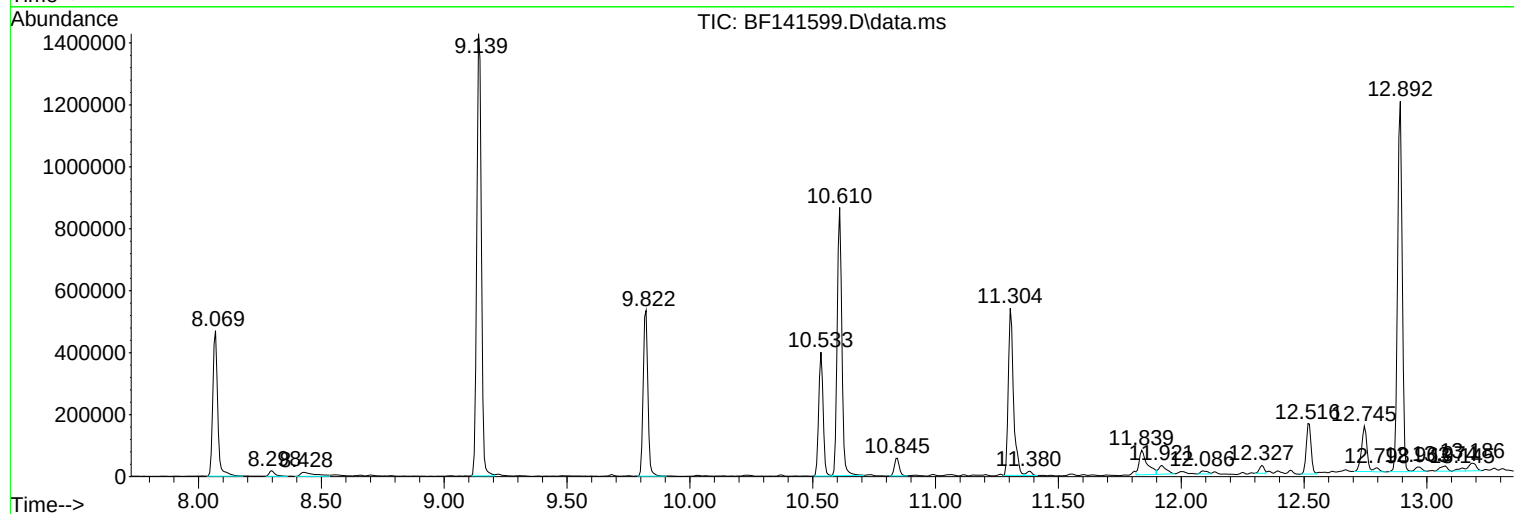
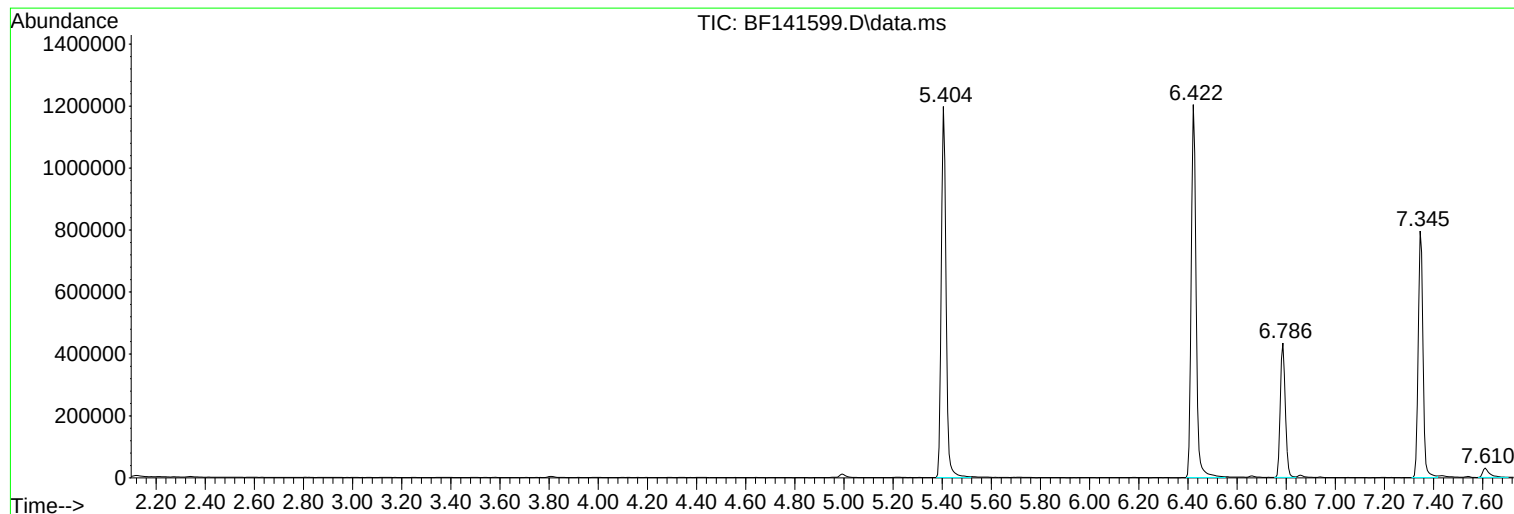
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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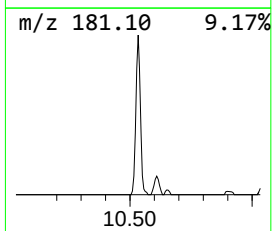
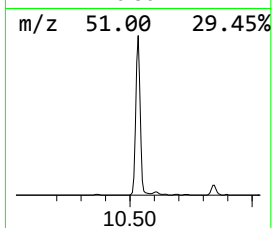
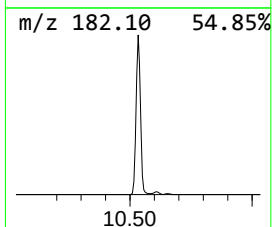
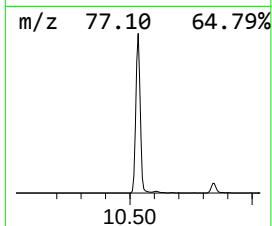
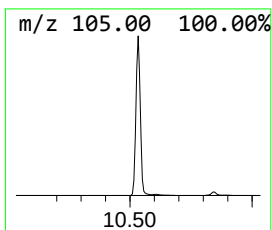
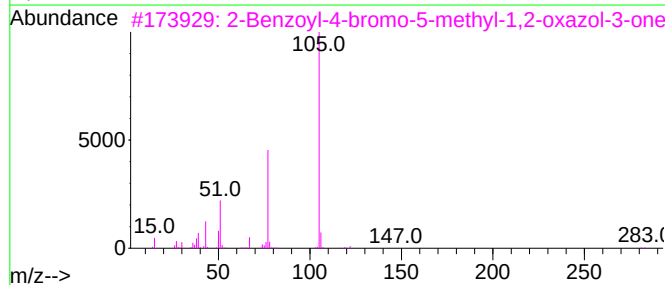
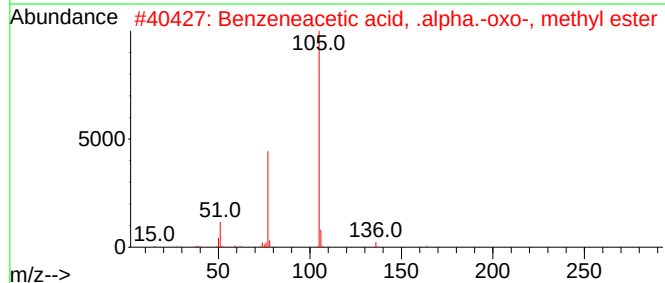
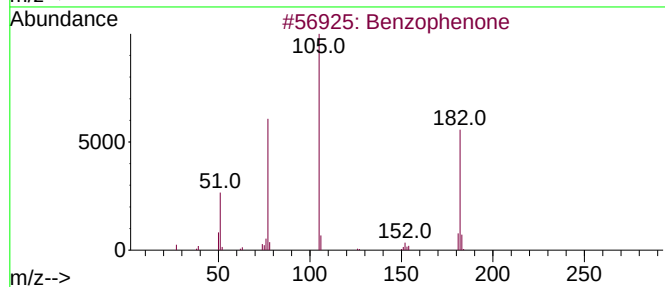
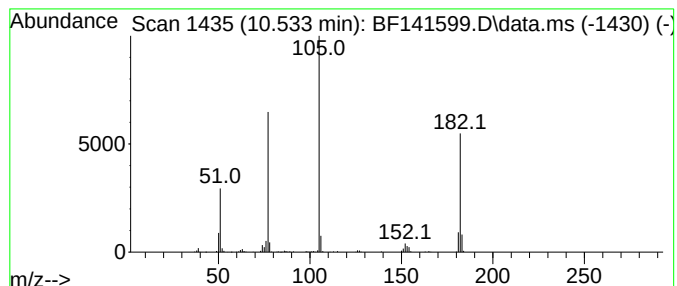
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	14.17 ng	502129	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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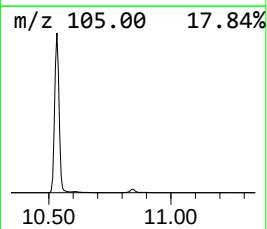
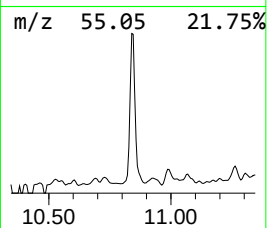
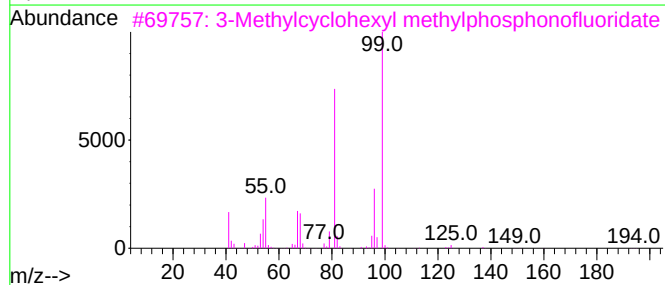
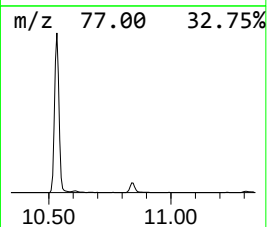
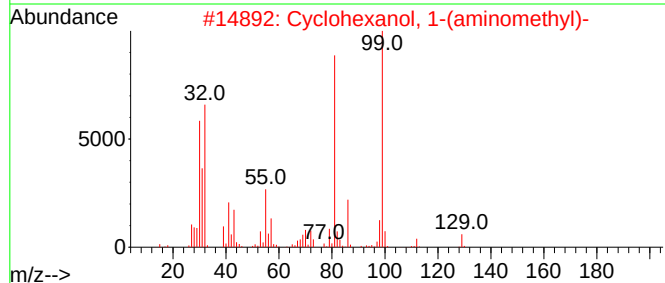
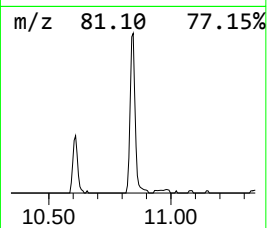
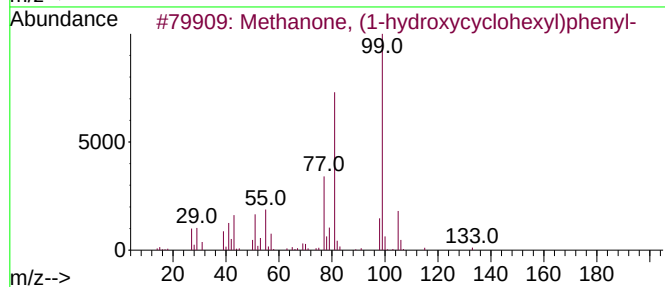
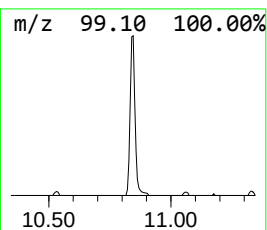
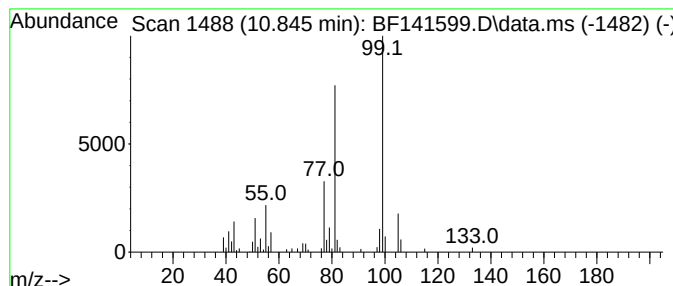
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Peak Number 2 Methanone, (1-hydroxycyclohexyl) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	2.01 ng	80291	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	59
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	42
4			2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	40
5			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	35



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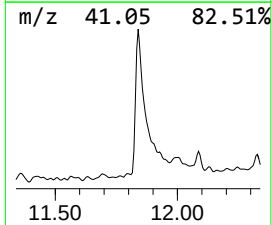
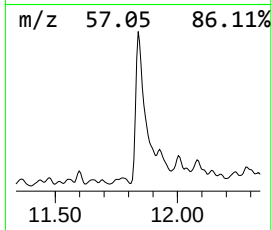
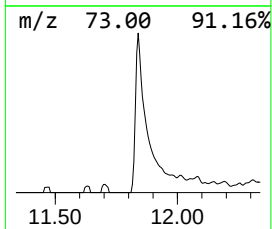
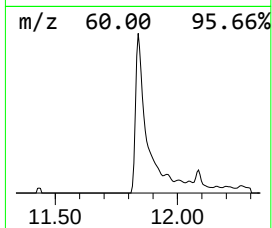
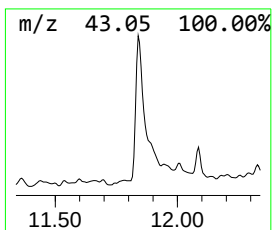
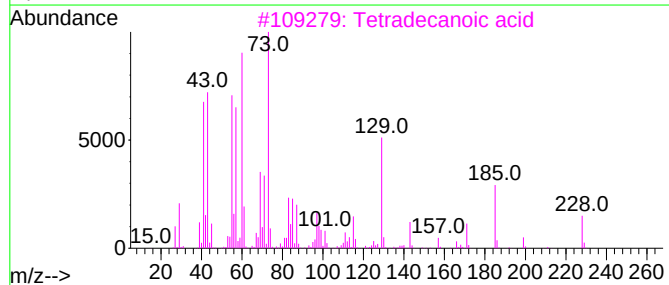
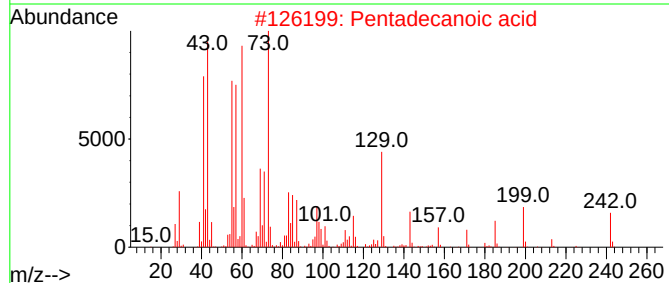
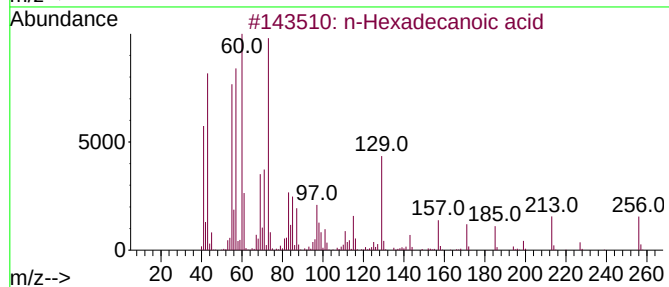
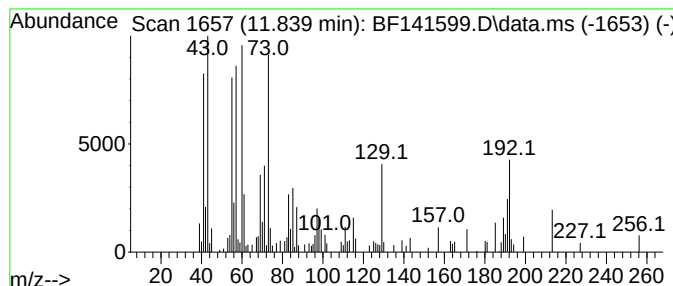
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.53 ng	180481	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15



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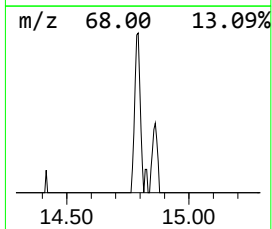
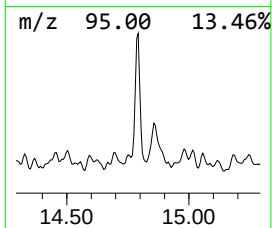
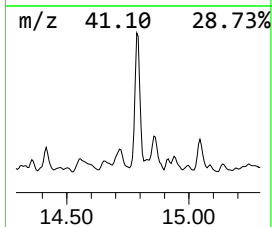
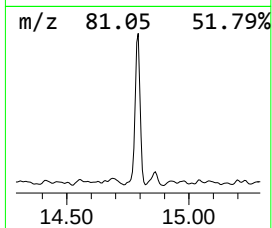
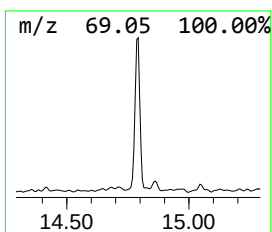
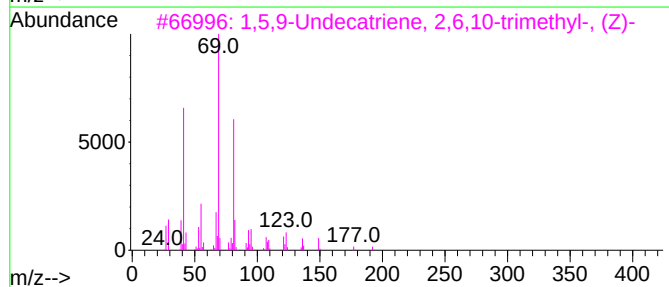
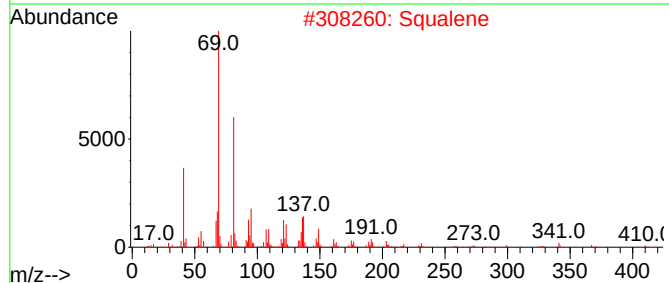
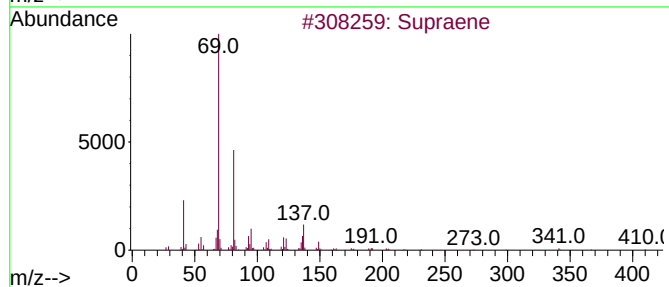
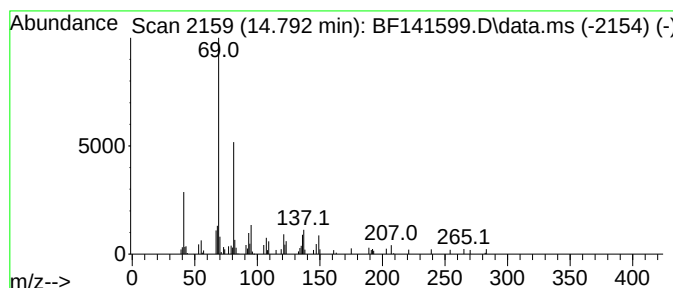
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	2.23 ng	50584	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Squalene	410	C30H50	000111-02-4	80
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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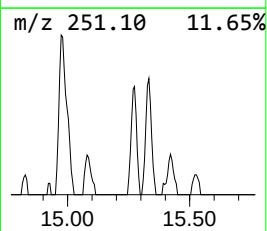
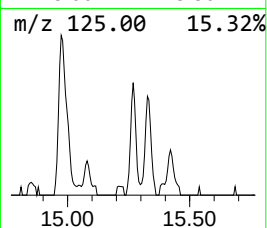
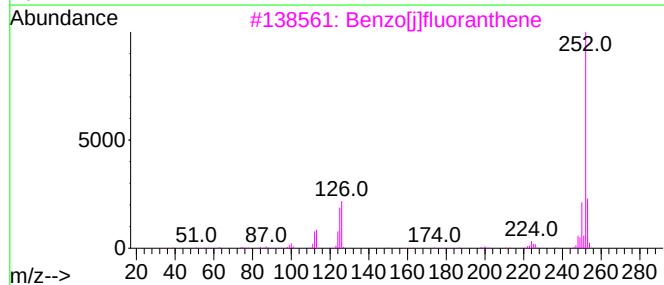
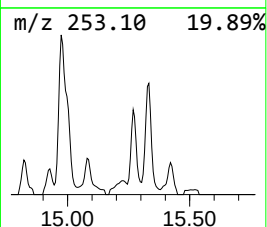
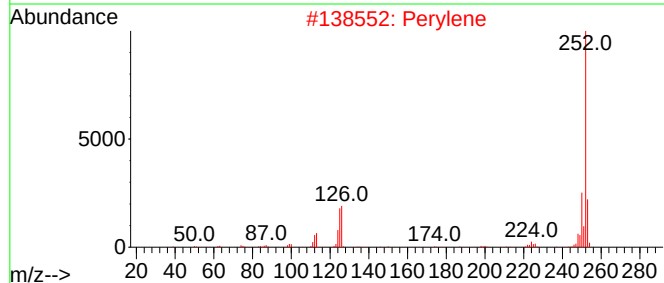
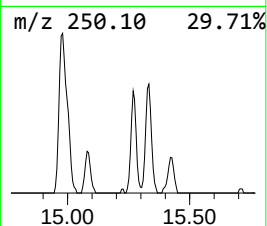
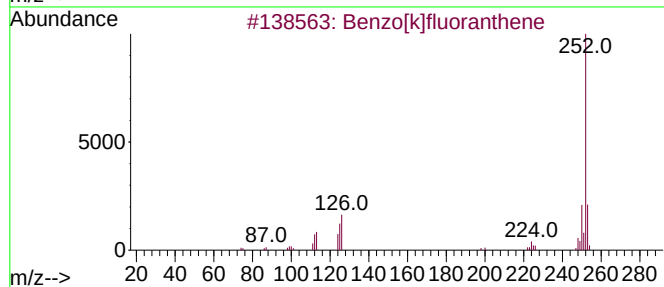
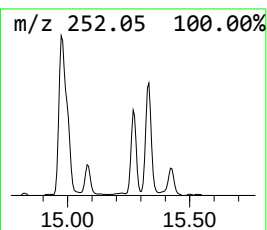
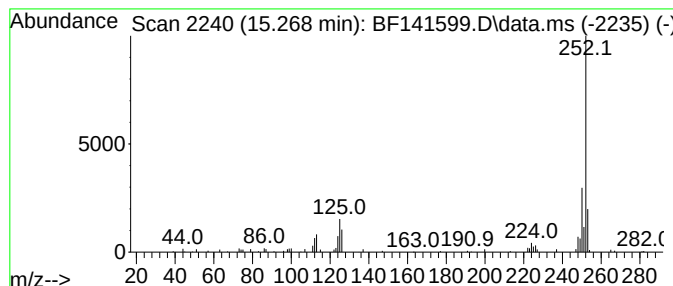
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.268	2.50 ng	56687	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[e]pyrene	252	C20H12	000192-97-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021225\
Data File : BF141599.D
Acq On : 12 Feb 2025 19:12
Operator : RC/JU
Sample : Q1343-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
Benzophenone	10.533	14.2	ng	502129	3	9.822	708628	20.0
Methanone, (1-h...	10.845	2.0	ng	80291	4	11.304	797673	20.0
n-Hexadecanoic ...	11.839	4.5	ng	180481	4	11.304	797673	20.0
Supraene	14.792	2.2	ng	50584	6	15.392	454073	20.0
Perylene	15.268	2.5	ng	56687	6	15.392	454073	20.0