

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
 Data File : BF137600.D
 Acq On : 14 Mar 2024 19:58
 Operator : CG\JU
 Sample : P1746-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-0-2.0

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.069	164	167	180	rBV2	37065	112286	3.04%	0.401%
2	5.334	548	552	567	rBV	3515833	3479958	94.26%	12.442%
3	6.363	722	727	748	rBV	3439171	3506847	94.98%	12.538%
4	6.728	785	789	804	rBV	833347	830595	22.50%	2.970%
5	7.287	881	884	896	rBV	2151167	2159441	58.49%	7.721%
6	8.004	1003	1006	1011	rBV	1187899	1016477	27.53%	3.634%
7	8.045	1011	1013	1027	rVB	69556	98879	2.68%	0.354%
8	8.328	1058	1061	1070	rBV	44014	71928	1.95%	0.257%
9	9.081	1185	1189	1201	rBV	4143877	3692020	100.00%	13.200%
10	9.622	1277	1281	1285	rVB	43391	42007	1.14%	0.150%
11	9.757	1300	1304	1315	rBV	1318958	1115317	30.21%	3.988%
12	9.857	1316	1321	1328	rVB2	76377	105912	2.87%	0.379%
13	10.545	1434	1438	1451	rBV	1856900	1842194	49.90%	6.586%
14	11.239	1552	1556	1558	rBV	1138408	932589	25.26%	3.334%
15	11.263	1558	1560	1564	rVB	160506	151521	4.10%	0.542%
16	11.639	1621	1624	1631	rVB2	37810	40124	1.09%	0.143%
17	11.775	1644	1647	1657	rBV3	218577	309474	8.38%	1.106%
18	12.445	1758	1761	1768	rBV	306499	306969	8.31%	1.097%
19	12.557	1776	1780	1784	rBV2	25314	51438	1.39%	0.184%
20	12.674	1794	1800	1804	rBV	306917	326622	8.85%	1.168%
21	12.763	1812	1815	1818	rVB	141452	112264	3.04%	0.401%
22	12.822	1821	1825	1829	rBV	3242499	2970753	80.46%	10.621%
23	13.057	1861	1865	1870	rBV3	28038	53428	1.45%	0.191%
24	13.110	1870	1874	1882	rVB2	45350	69397	1.88%	0.248%
25	13.398	1919	1923	1927	rBV4	52612	65956	1.79%	0.236%
26	13.727	1976	1979	1987	rBV2	200886	267431	7.24%	0.956%
27	13.869	1997	2003	2007	rBV2	1054286	1326656	35.93%	4.743%
28	13.898	2007	2008	2014	rVB	215622	163423	4.43%	0.584%
29	14.351	2082	2085	2087	rBV2	65786	67638	1.83%	0.242%
30	14.645	2132	2135	2138	rBV2	41683	45970	1.25%	0.164%
31	14.716	2144	2147	2150	rBV	76005	82697	2.24%	0.296%
32	14.786	2156	2159	2166	rVB4	62466	78373	2.12%	0.280%
33	14.886	2172	2176	2179	rBV	244207	342528	9.28%	1.225%
34	14.968	2187	2190	2192	rBV2	70766	81299	2.20%	0.291%
35	14.992	2192	2194	2201	rVB	50659	91084	2.47%	0.326%
36	15.174	2222	2225	2232	rVB	145474	173355	4.70%	0.620%

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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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.233	2232	2235	2241	rBV	190404	235658	6.38%	0.843%
38	15.292	2241	2245	2250	rBV	848557	1062155	28.77%	3.797%
39	15.739	2318	2321	2327	rVB	72235	90911	2.46%	0.325%
40	16.674	2476	2480	2490	rVB2	70315	146666	3.97%	0.524%
41	16.833	2502	2507	2514	rBV6	60074	130637	3.54%	0.467%
42	17.092	2546	2551	2558	rBV2	56707	119109	3.23%	0.426%

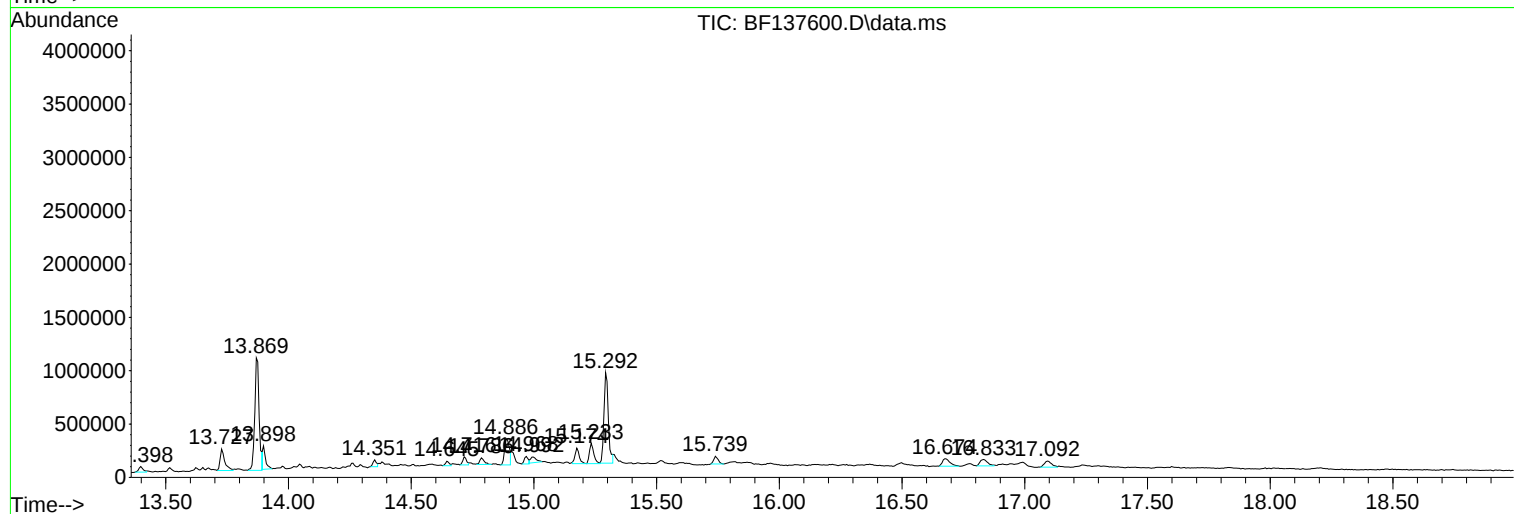
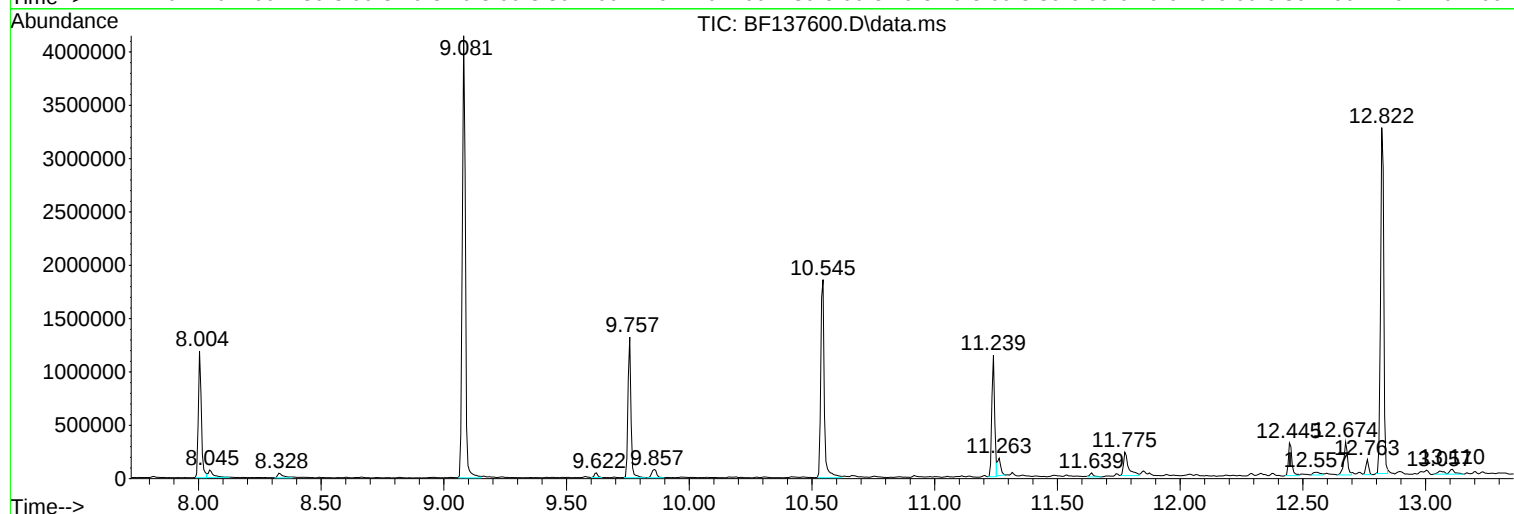
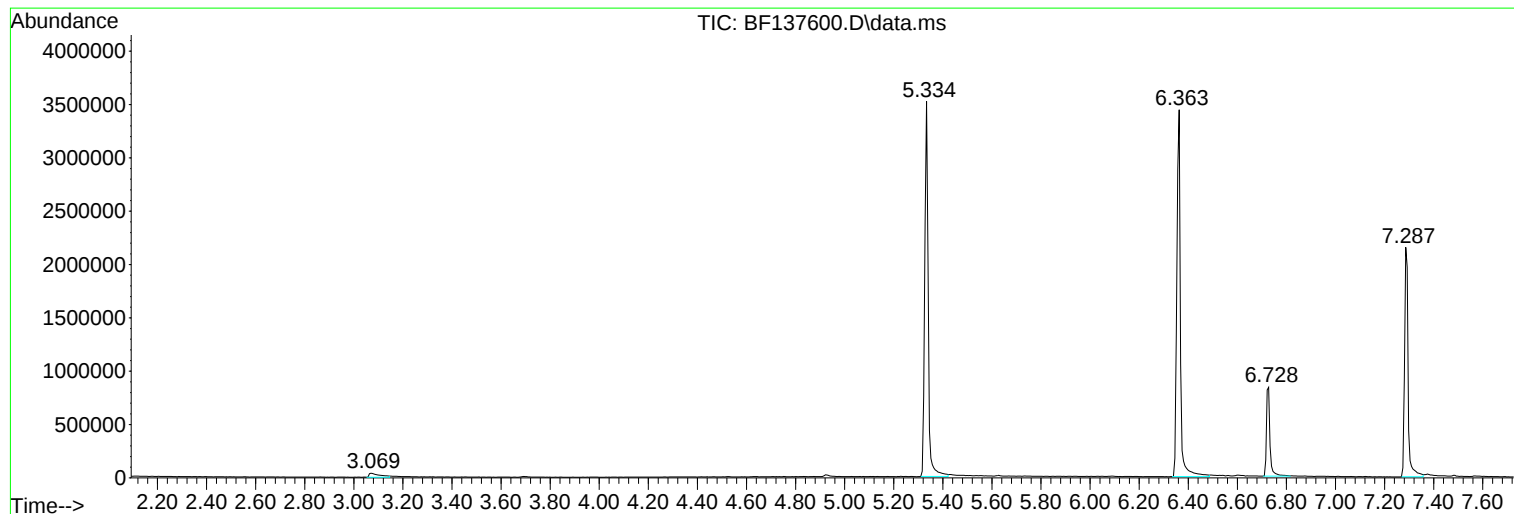
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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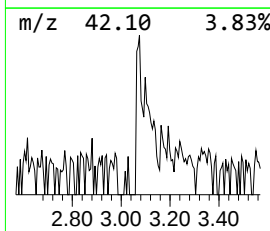
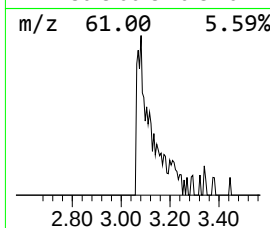
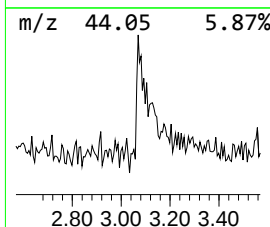
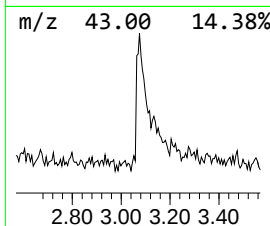
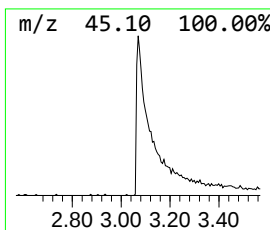
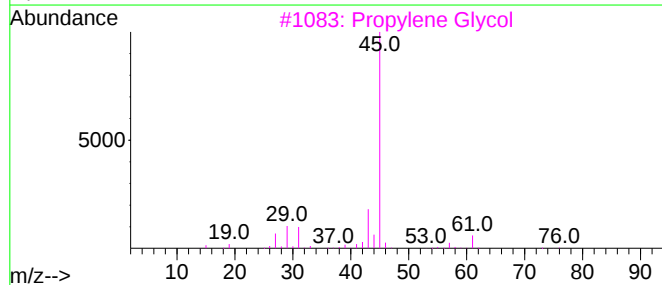
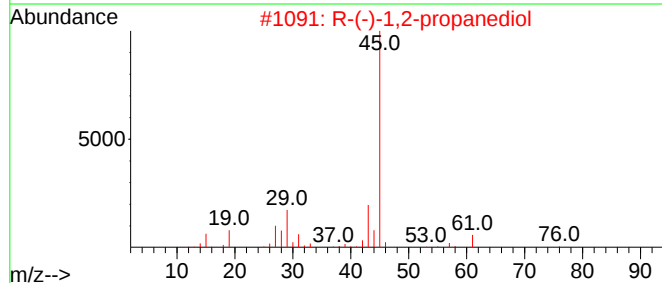
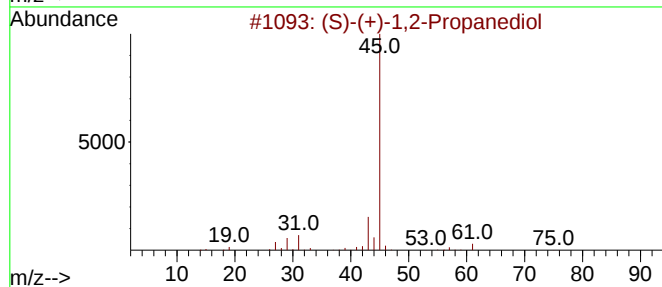
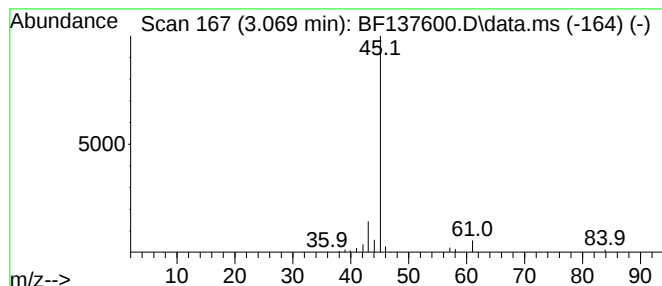
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.069	2.70 ng	112286	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	2-Pentanol			88	C5H12O	006032-29-7	9
5	2-Hexanol, (R)-			102	C6H14O	026549-24-6	9



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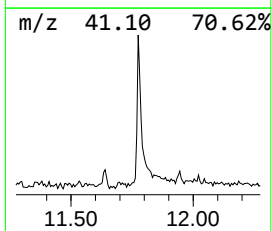
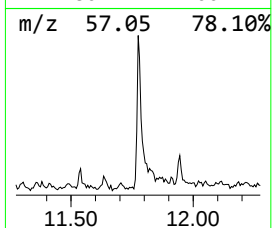
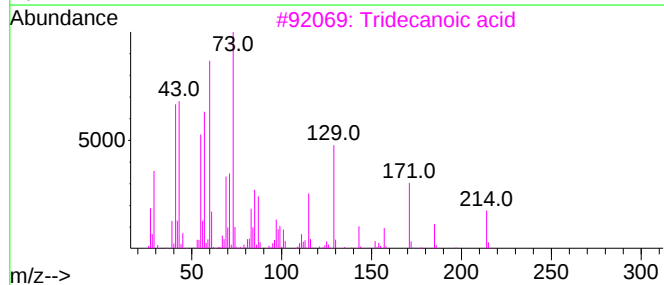
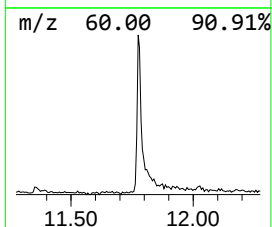
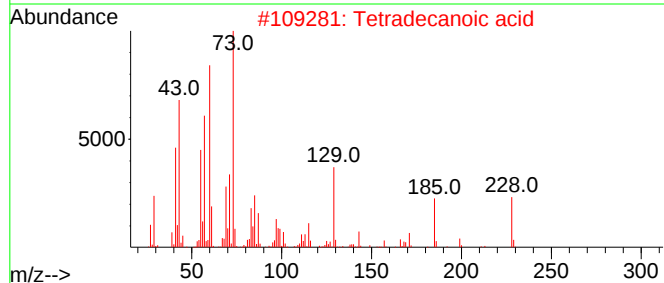
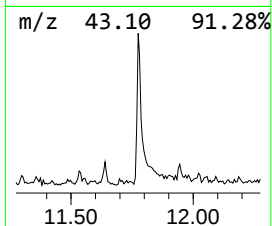
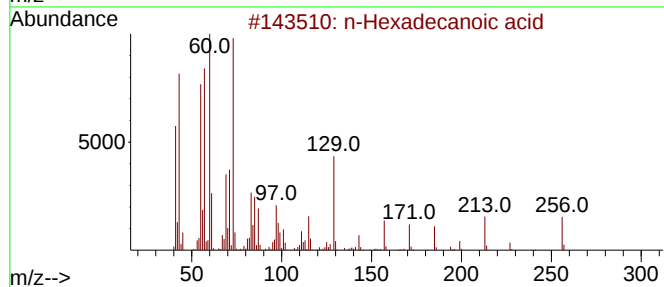
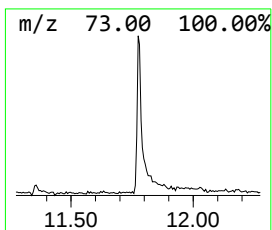
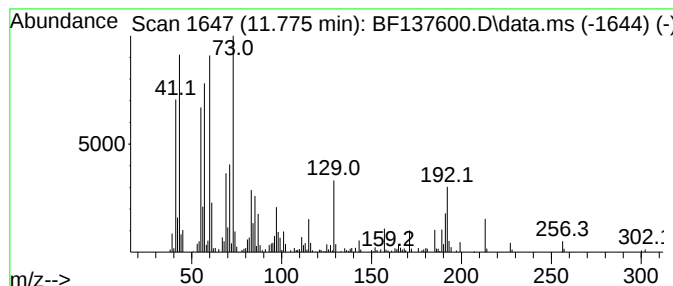
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	6.64 ng	309474	Phenanthrene-d10	11.239

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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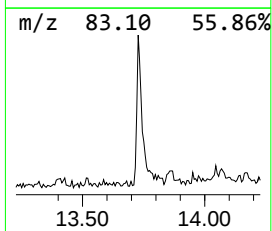
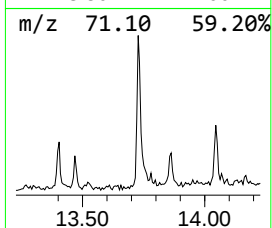
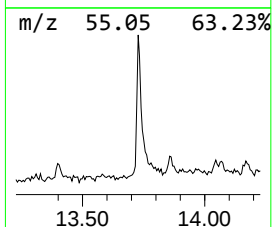
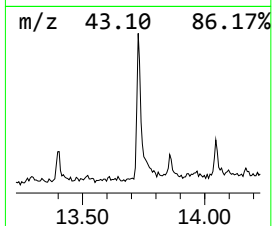
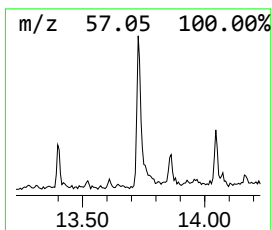
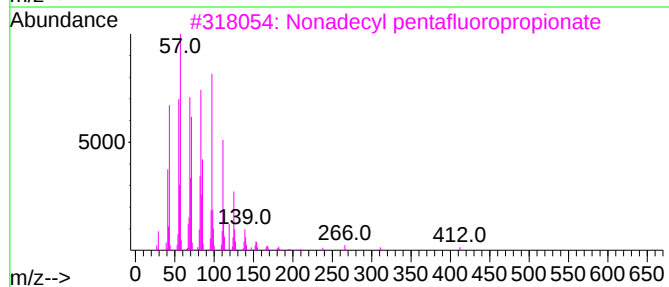
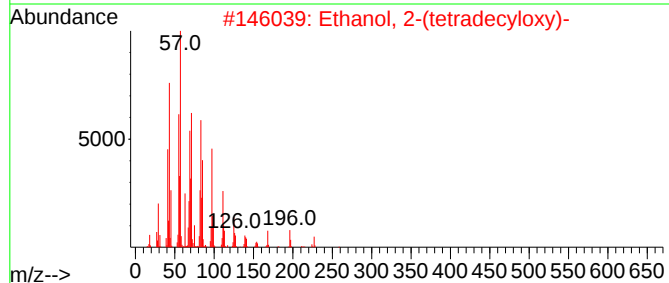
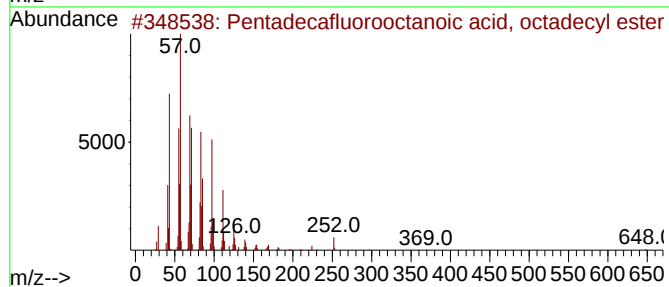
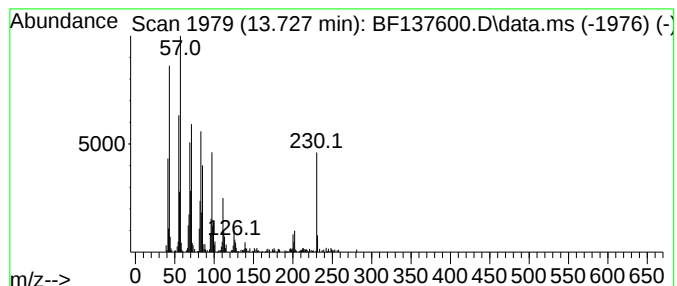
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.727	4.03 ng	267431	Chrysene-d12	13.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	89
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64



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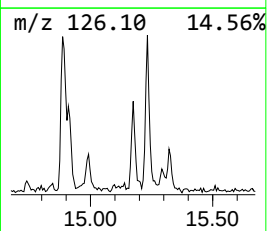
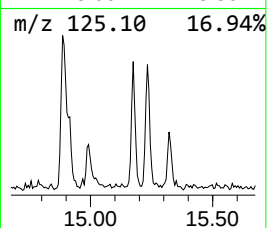
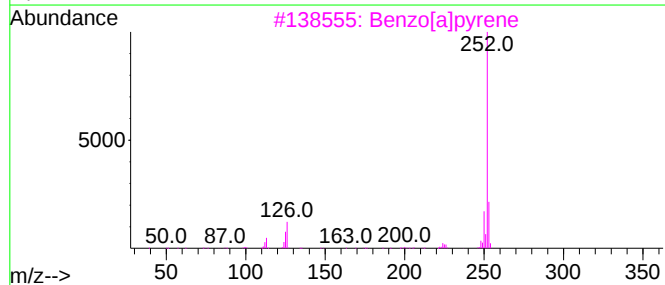
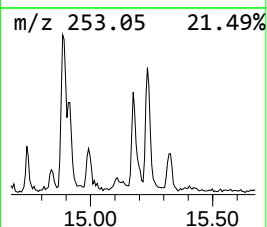
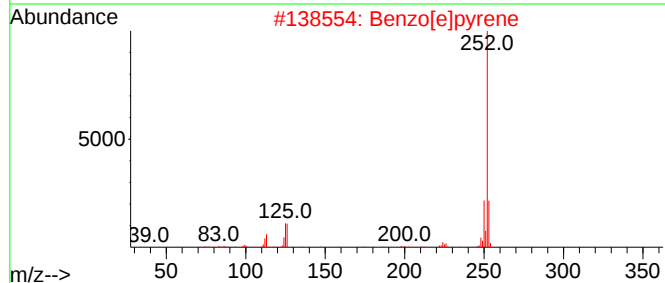
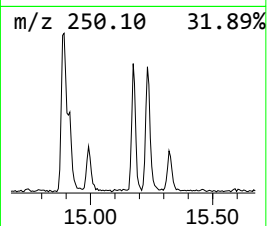
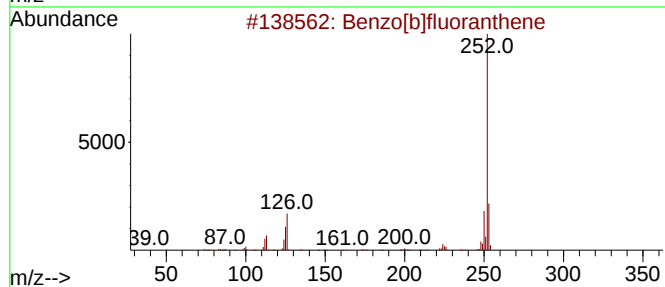
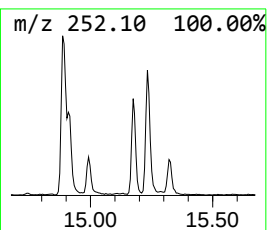
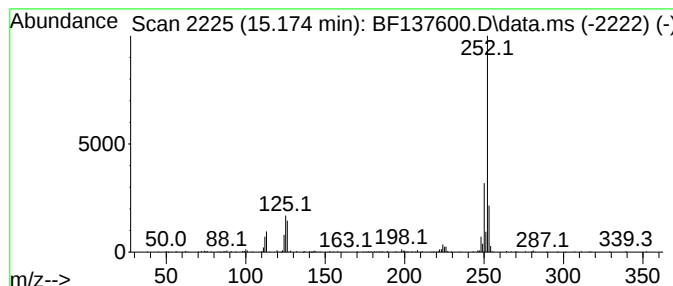
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.26 ng	173355	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5			Perylene	252	C20H12	000198-55-0	89



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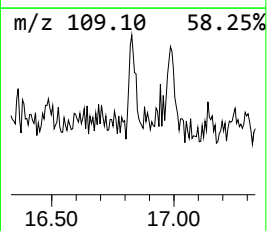
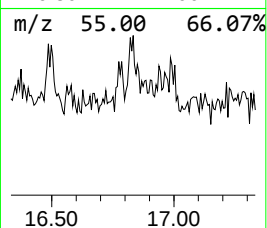
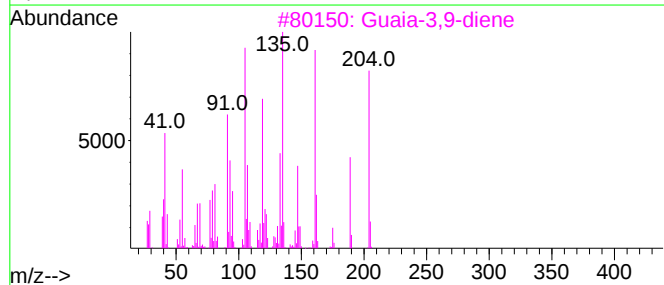
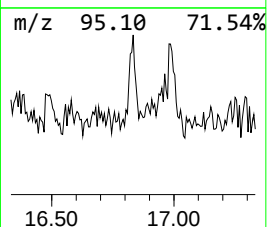
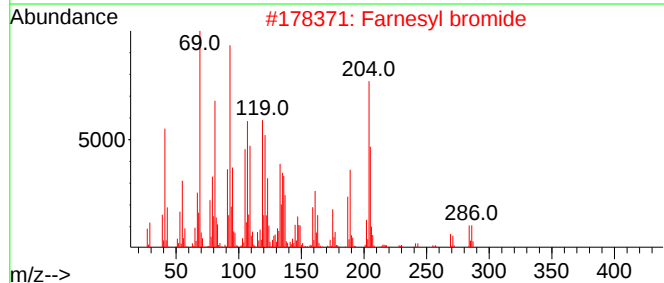
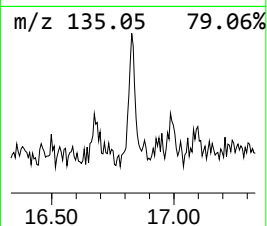
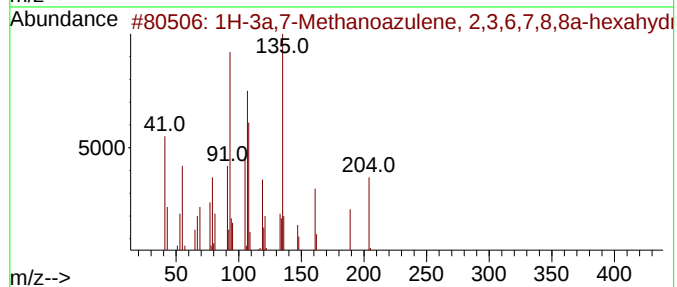
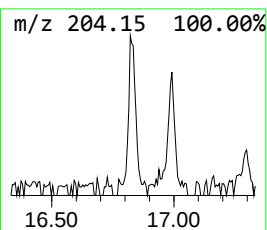
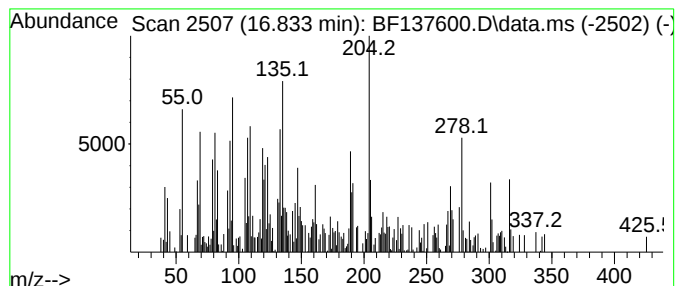
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.833	2.46 ng	130637	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	50
2			Farnesyl bromide	284	C15H25Br	006874-67-5	46
3			Guaia-3,9-diene	204	C15H24	000489-83-8	41
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	38
5			cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137600.D
Acq On : 14 Mar 2024 19:58
Operator : CG\JU
Sample : P1746-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
(S)-(+)-1,2-Pro...	3.069	2.7	ng	112286	1	6.728	830595	20.0
n-Hexadecanoic ...	11.775	6.6	ng	309474	4	11.239	932589	20.0
Pentadecafluoro...	13.727	4.0	ng	267431	5	13.874	1326660	20.0
Benzo[e]pyrene	15.174	3.3	ng	173355	6	15.292	1062160	20.0
1H-3a,7-Methano...	16.833	2.5	ng	130637	6	15.292	1062160	20.0