

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
 Data File : BF135737.D
 Acq On : 12 Oct 2023 16:28
 Operator : CG\JU
 Sample : 04837-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-284

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	487	491	501	rBV	76734	120101	6.16%	0.784%
2	5.375	556	559	586	rBV	1771977	1951114	100.00%	12.738%
3	6.387	728	731	750	rBV	1610000	1838777	94.24%	12.005%
4	6.598	764	767	774	rBV2	9560	21108	1.08%	0.138%
5	6.740	787	791	801	rVB	621798	563998	28.91%	3.682%
6	7.304	884	887	899	rBV	1295045	1188253	60.90%	7.758%
7	8.016	1005	1008	1017	rBV	788859	691838	35.46%	4.517%
8	9.092	1188	1191	1198	rBV	1942877	1675538	85.88%	10.939%
9	9.216	1208	1212	1216	rVB2	31597	32613	1.67%	0.213%
10	9.775	1303	1307	1319	rBV	847549	711936	36.49%	4.648%
11	10.569	1439	1442	1455	rBV	983554	988921	50.68%	6.456%
12	11.269	1558	1561	1564	rBV	701033	643267	32.97%	4.200%
13	11.292	1564	1565	1571	rVV	193649	167853	8.60%	1.096%
14	11.351	1571	1575	1581	rVB	37454	42944	2.20%	0.280%
15	11.522	1601	1604	1610	rBV3	17986	25800	1.32%	0.168%
16	11.774	1645	1647	1650	rBV	30806	27813	1.43%	0.182%
17	11.804	1650	1652	1659	rVV3	134070	147005	7.53%	0.960%
18	11.886	1663	1666	1669	rBV2	43792	49623	2.54%	0.324%
19	12.074	1695	1698	1702	rVB	27223	22273	1.14%	0.145%
20	12.327	1738	1741	1744	rBV2	28559	28241	1.45%	0.184%
21	12.427	1756	1758	1761	rVB3	19474	19881	1.02%	0.130%
22	12.492	1766	1769	1775	rBV	390454	340578	17.46%	2.224%
23	12.592	1784	1786	1792	rBV2	28676	41055	2.10%	0.268%
24	12.645	1792	1795	1798	rVV2	23206	23162	1.19%	0.151%
25	12.721	1802	1808	1813	rVV	307935	348680	17.87%	2.276%
26	12.863	1828	1832	1836	rBV	1269407	1128646	57.85%	7.369%
27	12.951	1842	1847	1851	rBV4	22395	42345	2.17%	0.276%
28	13.027	1858	1860	1863	rBV3	20299	27192	1.39%	0.178%
29	13.057	1863	1865	1868	rVB3	38641	34913	1.79%	0.228%
30	13.163	1879	1883	1887	rBV3	35530	46888	2.40%	0.306%
31	13.292	1901	1905	1911	rBV6	24010	32938	1.69%	0.215%
32	13.439	1926	1930	1932	rBV2	24406	23242	1.19%	0.152%
33	13.580	1952	1954	1960	rVB	26795	27056	1.39%	0.177%
34	13.686	1969	1972	1973	rBV	28019	23081	1.18%	0.151%
35	13.704	1973	1975	1978	rVB2	28281	28811	1.48%	0.188%
36	13.739	1978	1981	1982	rBV	19826	20631	1.06%	0.135%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
 Data File : BF135737.D
 Acq On : 12 Oct 2023 16:28
 Operator : CG\JU
 Sample : 04837-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-284

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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.792	1988	1990	1996	rVB2	29474	36208	1.86%	0.236%
38	13.868	1996	2003	2005	rBV4	22692	50776	2.60%	0.331%
39	13.933	2007	2014	2017	rVV2	556130	670285	34.35%	4.376%
40	13.957	2017	2018	2022	rVB	133194	117834	6.04%	0.769%
41	14.039	2030	2032	2035	rVB	23349	20263	1.04%	0.132%
42	14.086	2037	2040	2048	rBV5	27113	53283	2.73%	0.348%
43	14.327	2076	2081	2085	rBV	36942	46704	2.39%	0.305%
44	14.398	2089	2093	2096	rBV2	35915	45916	2.35%	0.300%
45	14.557	2118	2120	2128	rVB7	21850	27078	1.39%	0.177%
46	14.768	2153	2156	2162	rVB	142951	143900	7.38%	0.939%
47	14.980	2188	2192	2195	rBV	108526	156418	8.02%	1.021%
48	15.092	2208	2211	2218	rVB	26275	38263	1.96%	0.250%
49	15.286	2240	2244	2248	rBV	62398	76685	3.93%	0.501%
50	15.351	2251	2255	2260	rVV	85595	102334	5.24%	0.668%
51	15.404	2260	2264	2278	rVB	333854	483012	24.76%	3.153%
52	15.839	2336	2338	2347	rVB10	15586	22341	1.15%	0.146%
53	16.915	2517	2521	2530	rVB3	31994	77751	3.98%	0.508%

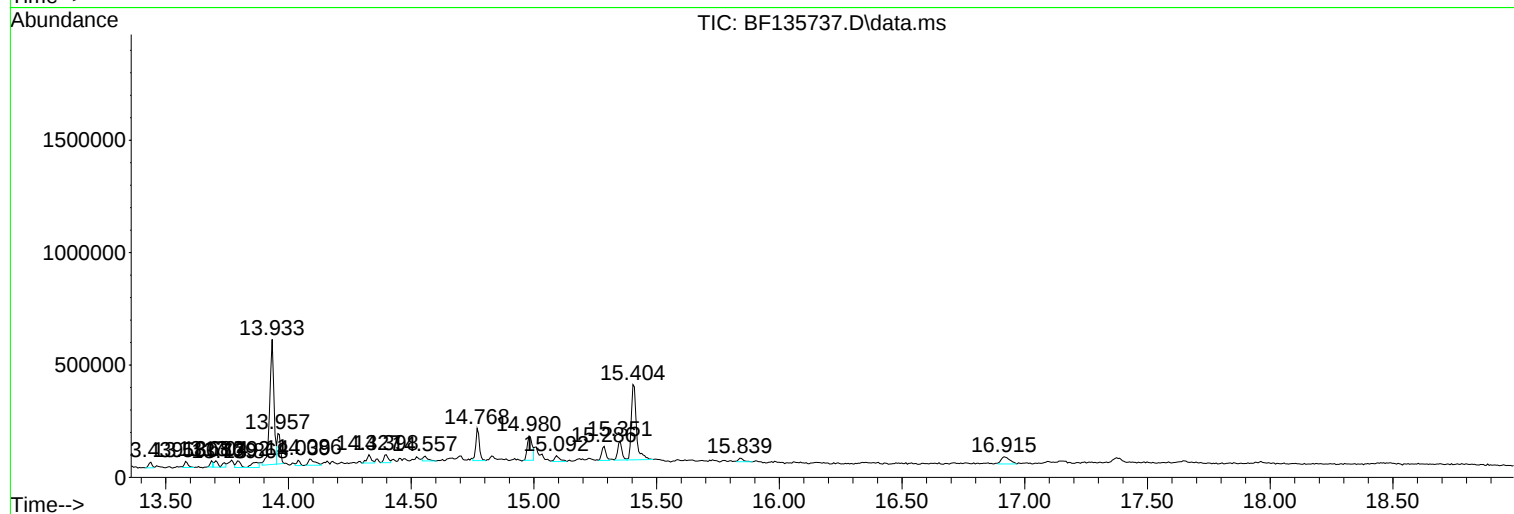
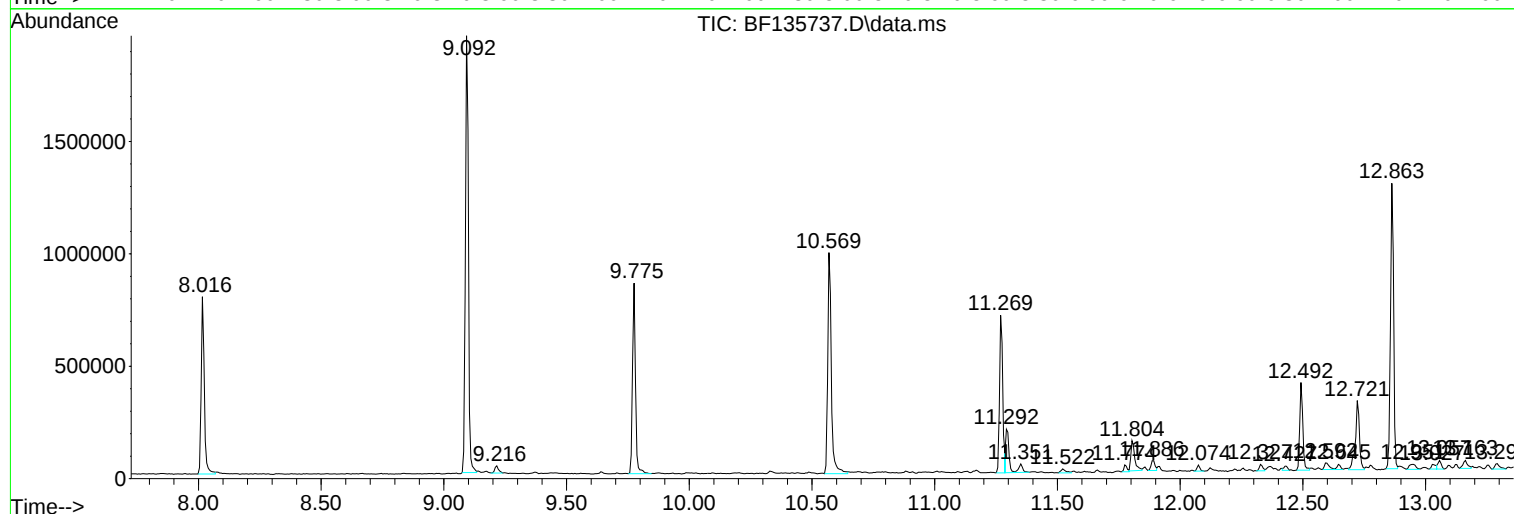
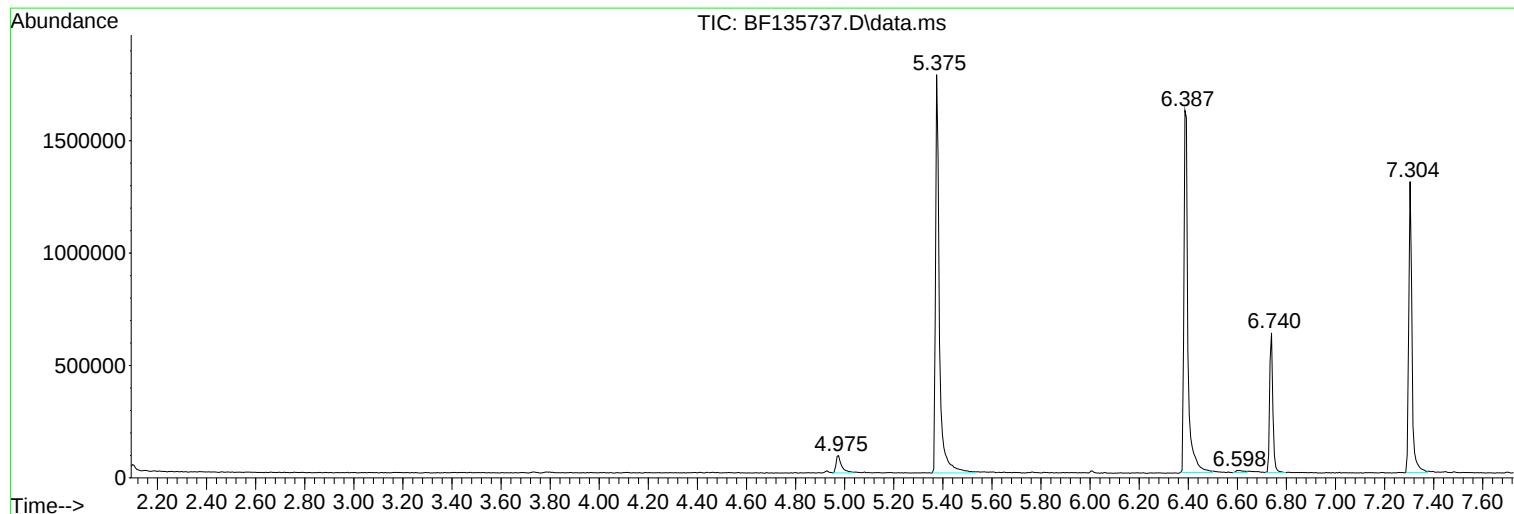
Sum of corrected areas: 15317166

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-284

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

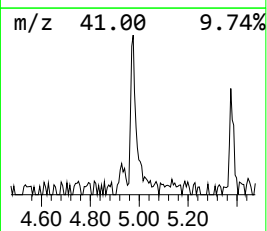
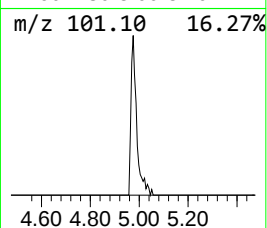
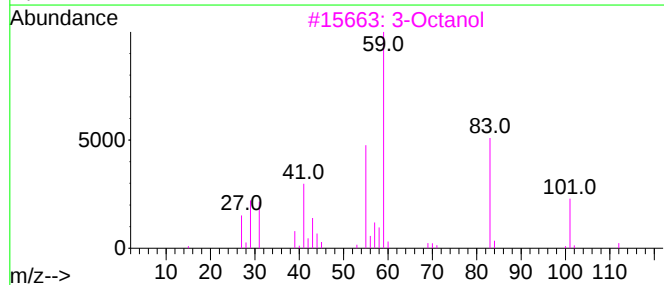
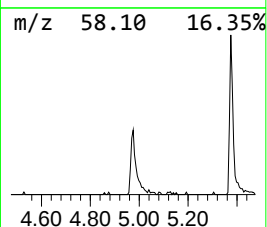
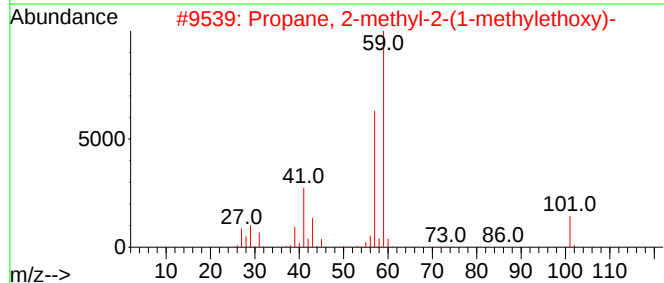
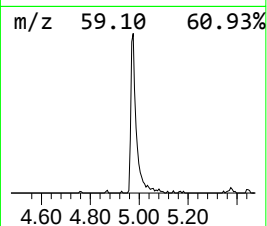
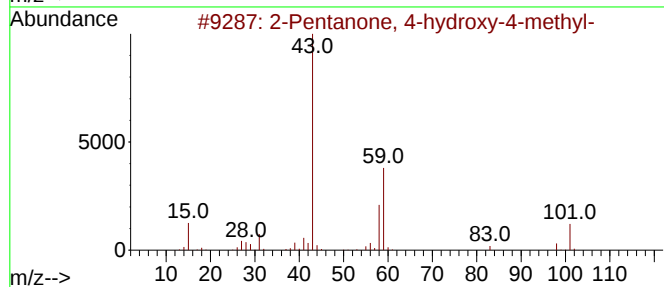
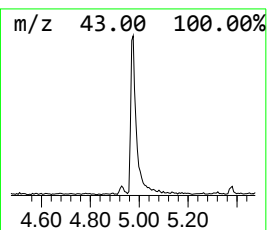
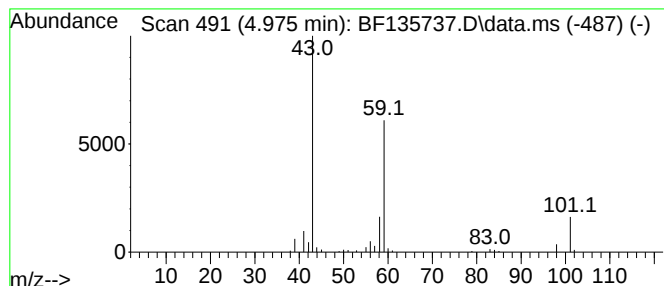
Instrument :
BNA_F
ClientSampleId :
ETGI-284

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.975	4.26 ng	120101	1,4-Dichlorobenzene-d4			6.740
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	33
3	3-Octanol		130	C8H18O	000589-98-0	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

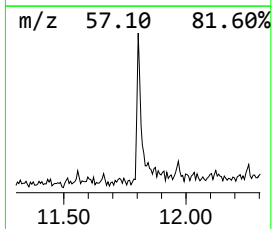
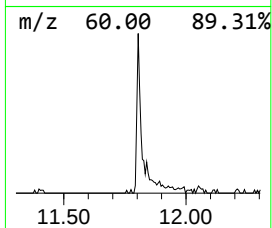
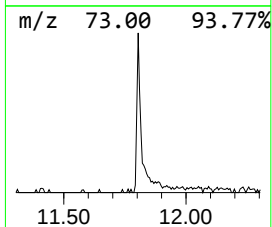
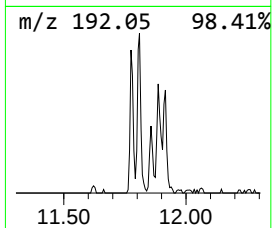
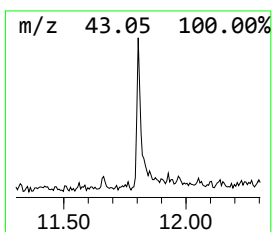
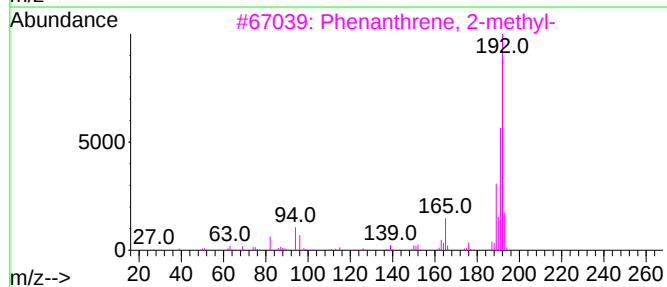
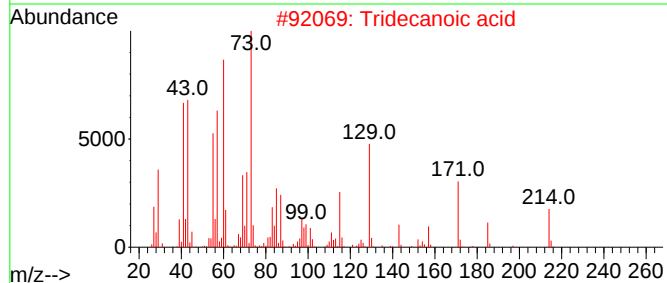
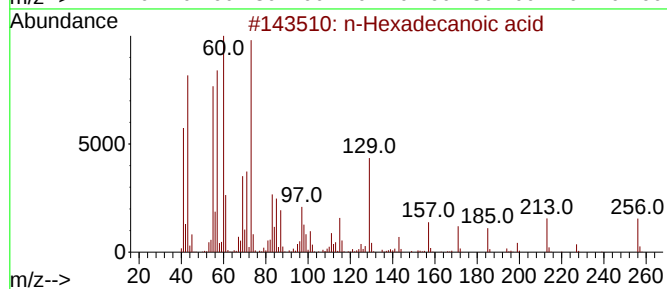
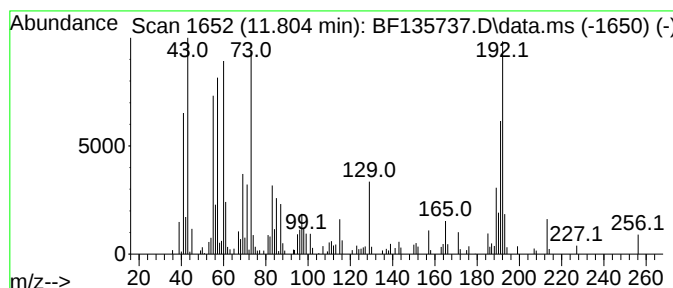
Instrument :
BNA_F
ClientSampleId :
ETGI-284

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.804	4.57 ng	147005	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-284

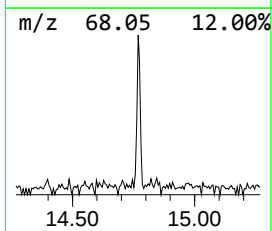
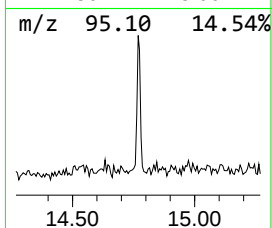
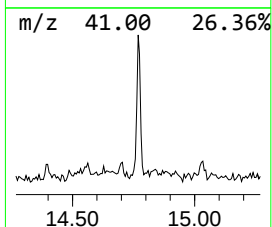
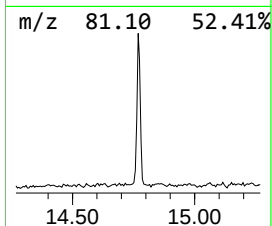
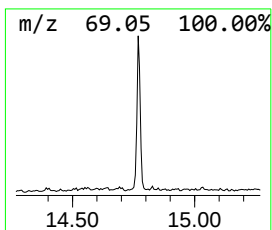
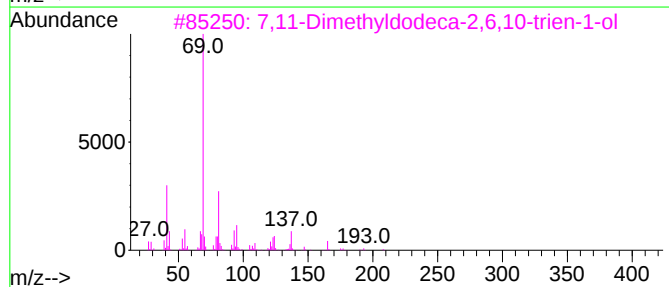
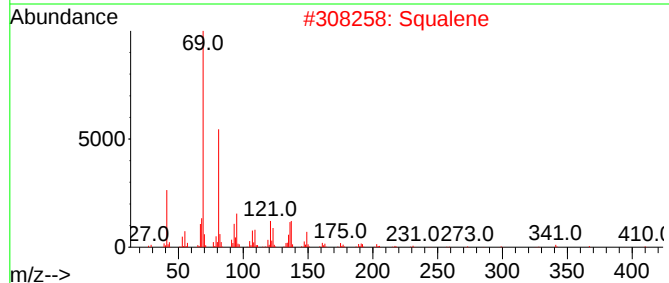
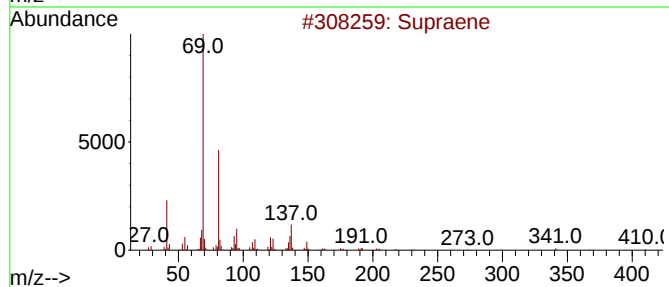
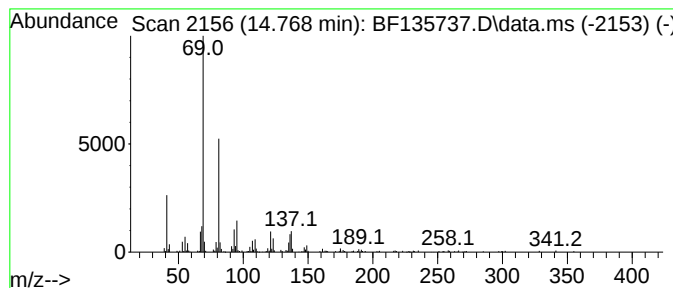
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	5.96 ng	143900	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-284

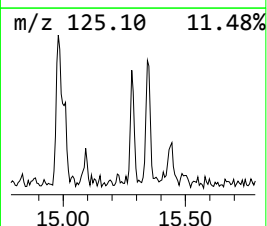
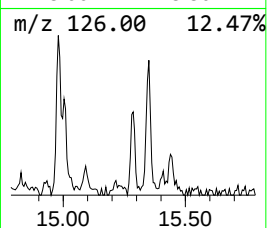
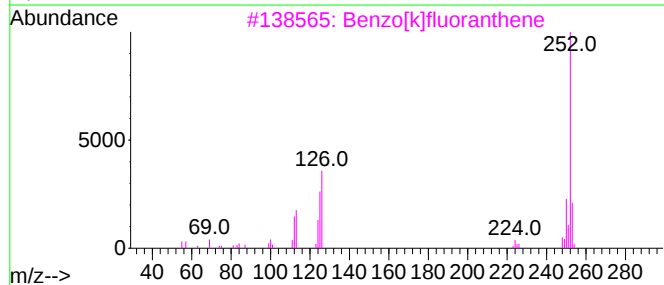
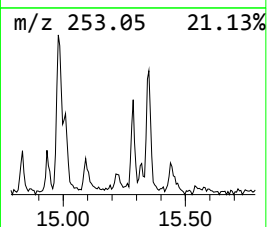
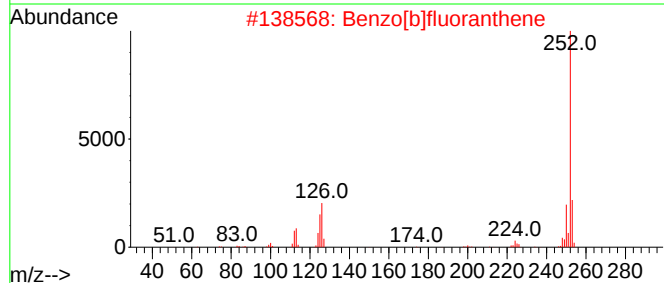
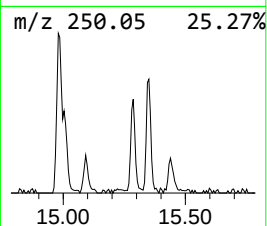
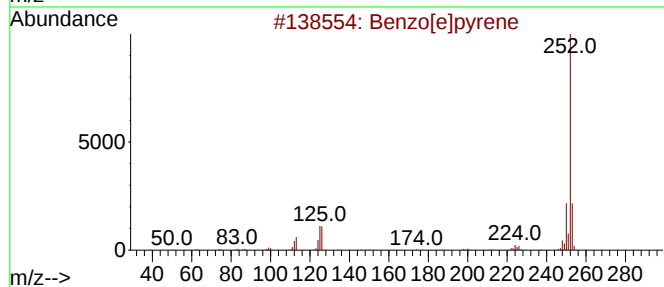
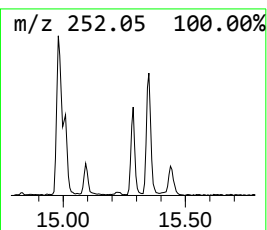
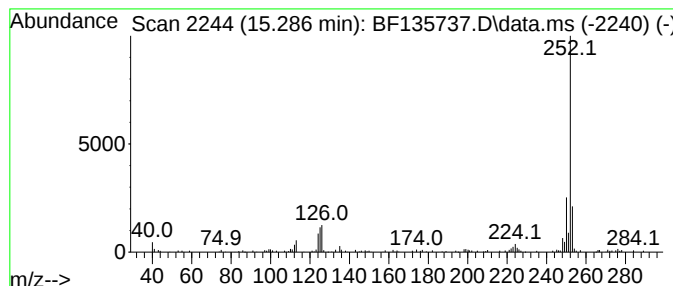
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	3.18 ng	76685	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101223\
Data File : BF135737.D
Acq On : 12 Oct 2023 16:28
Operator : CG\JU
Sample : 04837-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-284

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-Pentanone, 4-...	4.975	4.3	ng	120101	1	6.740	563998	20.0
n-Hexadecanoic ...	11.804	4.6	ng	147005	4	11.269	643267	20.0
Supraene	14.768	6.0	ng	143900	6	15.404	483012	20.0
Benzo[e]pyrene	15.286	3.2	ng	76685	6	15.404	483012	20.0