

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
 Data File : BF137608.D
 Acq On : 14 Mar 2024 23:47
 Operator : CG\JU
 Sample : P1746-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-0-2.0

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: BF137608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	548	552	574	rBV	2386204	2568183	96.57%	10.978%
2	6.363	723	727	745	rBV	2425479	2492383	93.72%	10.654%
3	6.728	785	789	808	rBV	795666	766817	28.83%	3.278%
4	7.287	881	884	896	rBV	1519873	1476922	55.53%	6.314%
5	8.004	1003	1006	1013	rBV	942140	889782	33.46%	3.804%
6	9.081	1186	1189	1201	rBV	3039804	2552253	95.97%	10.910%
7	9.622	1278	1281	1289	rBV	67515	66469	2.50%	0.284%
8	9.757	1300	1304	1308	rBV	1180322	940191	35.35%	4.019%
9	10.545	1434	1438	1452	rBV	1448868	1383280	52.01%	5.913%
10	11.239	1553	1556	1559	rBV	1082459	939751	35.34%	4.017%
11	11.263	1559	1560	1565	rVV	208240	155913	5.86%	0.666%
12	11.316	1566	1569	1573	rVB	41028	44512	1.67%	0.190%
13	11.486	1591	1598	1605	rBV5	20175	49757	1.87%	0.213%
14	11.745	1638	1642	1644	rBV	28624	30854	1.16%	0.132%
15	11.775	1644	1647	1652	rBV2	144122	183361	6.89%	0.784%
16	11.851	1657	1660	1663	rBV	43082	43953	1.65%	0.188%
17	12.292	1732	1735	1737	rBV	37301	40258	1.51%	0.172%
18	12.327	1738	1741	1746	rVB5	26079	42663	1.60%	0.182%
19	12.374	1746	1749	1754	rBV3	32786	40469	1.52%	0.173%
20	12.451	1758	1762	1767	rBV	491471	442340	16.63%	1.891%
21	12.545	1776	1778	1785	rBV	38702	70081	2.64%	0.300%
22	12.674	1794	1800	1804	rBV	462908	475546	17.88%	2.033%
23	12.727	1807	1809	1814	rVV3	30972	32205	1.21%	0.138%
24	12.827	1822	1826	1829	rBV	3000546	2659522	100.00%	11.369%
25	12.898	1834	1838	1843	rVB2	37651	51782	1.95%	0.221%
26	12.986	1850	1853	1854	rBV2	36028	39498	1.49%	0.169%
27	13.004	1854	1856	1860	rVB	64154	66123	2.49%	0.283%
28	13.074	1863	1868	1870	rVV2	38695	59622	2.24%	0.255%
29	13.110	1871	1874	1878	rVB	65514	65530	2.46%	0.280%
30	13.204	1887	1890	1893	rVB	35820	35474	1.33%	0.152%
31	13.233	1893	1895	1897	rBV	36288	36005	1.35%	0.154%
32	13.404	1921	1924	1926	rBV3	37696	33191	1.25%	0.142%
33	13.516	1940	1943	1948	rVB	50419	57576	2.16%	0.246%
34	13.621	1959	1961	1964	rBV2	38162	41511	1.56%	0.177%
35	13.727	1976	1979	1986	rBV2	186612	247719	9.31%	1.059%
36	13.874	1999	2004	2007	rBV2	1244706	1456771	54.78%	6.227%

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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	13.898	2007	2008	2014	rVB	293142	258416	9.72%	1.105%
38	13.980	2020	2022	2024	rVB	52411	40651	1.53%	0.174%
39	14.021	2027	2029	2031	rBV2	33790	33340	1.25%	0.143%
40	14.045	2031	2033	2036	rVB3	44780	46948	1.77%	0.201%
41	14.263	2068	2070	2073	rVB	57536	44594	1.68%	0.191%
42	14.357	2083	2086	2088	rBV2	73142	75613	2.84%	0.323%
43	14.721	2145	2148	2151	rBV2	107525	109728	4.13%	0.469%
44	14.892	2173	2177	2185	rBV	345964	623833	23.46%	2.667%
45	14.968	2188	2190	2192	rBV2	54599	47662	1.79%	0.204%
46	15.180	2223	2226	2232	rVB	173677	209607	7.88%	0.896%
47	15.239	2232	2236	2242	rBV	258501	341383	12.84%	1.459%
48	15.298	2242	2246	2250	rBV	664544	819889	30.83%	3.505%
49	17.104	2548	2553	2561	rVB	75865	163112	6.13%	0.697%

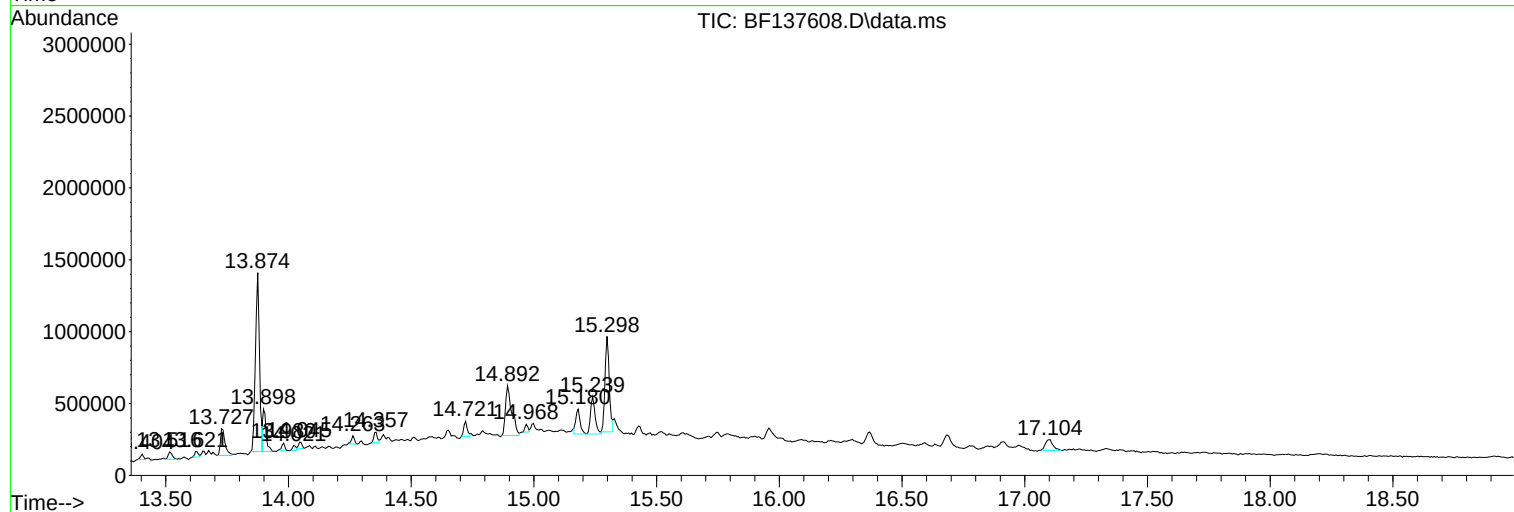
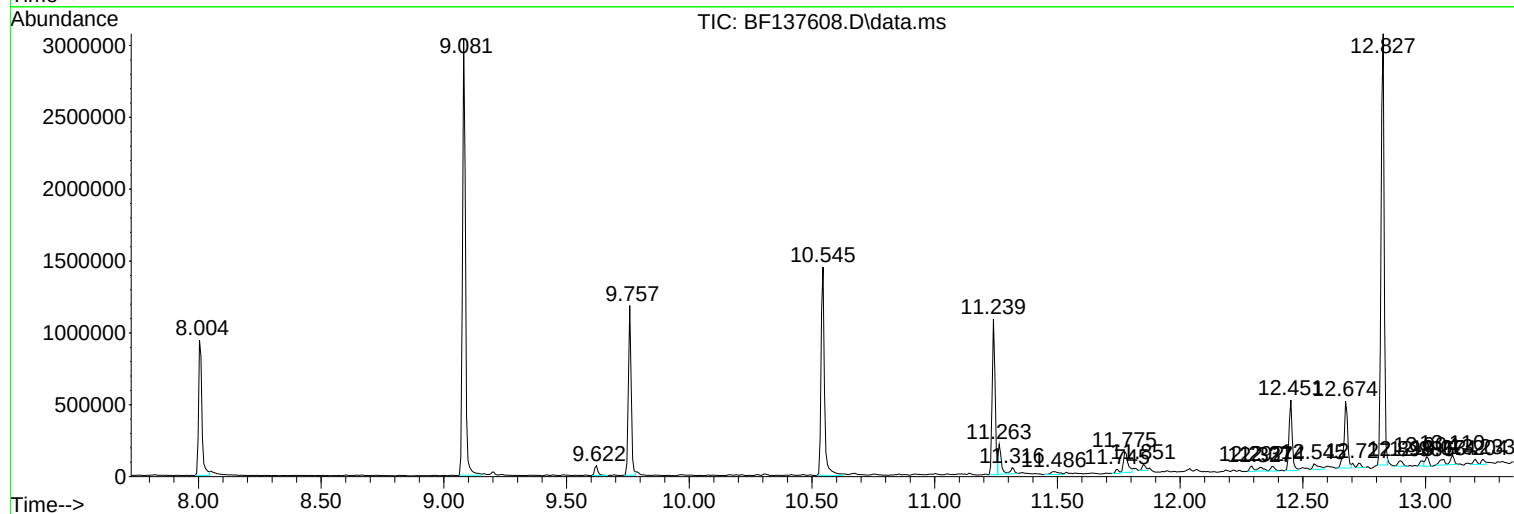
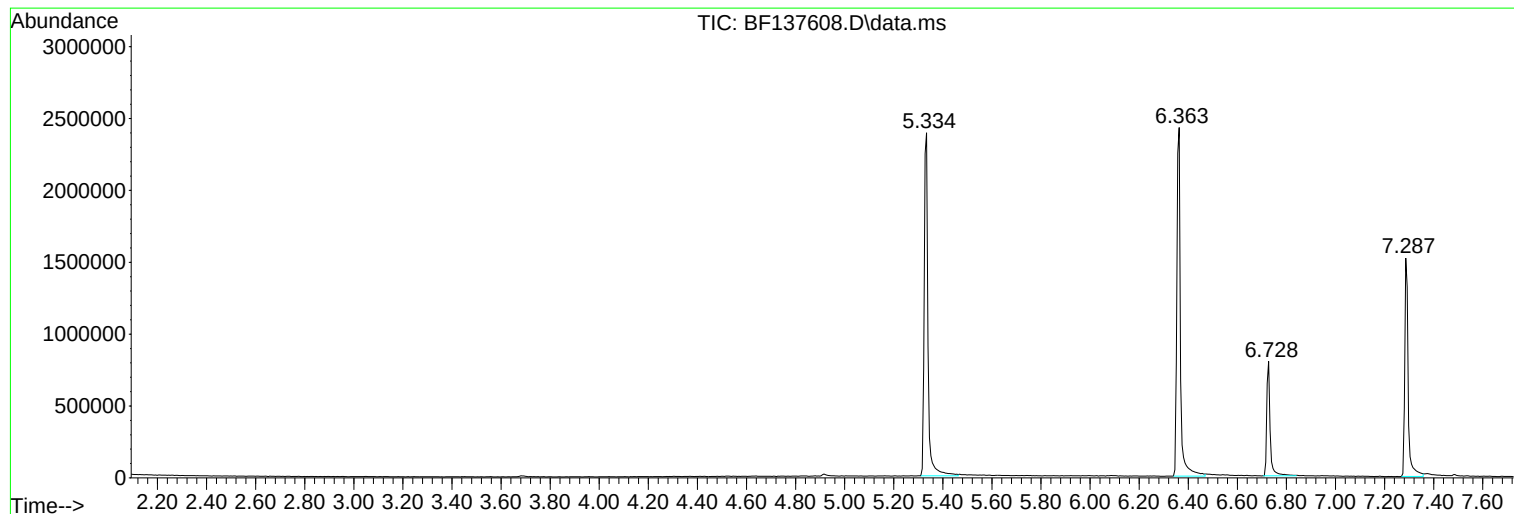
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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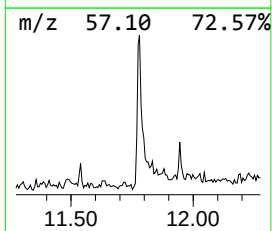
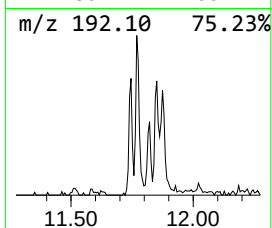
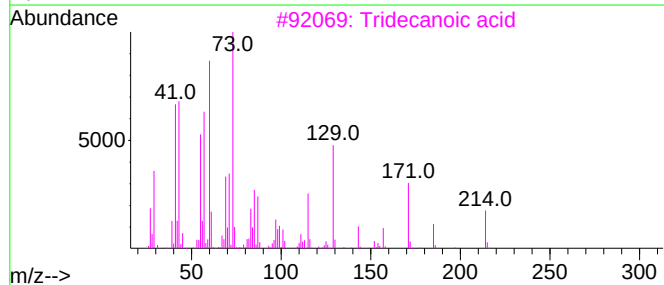
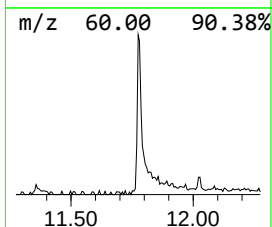
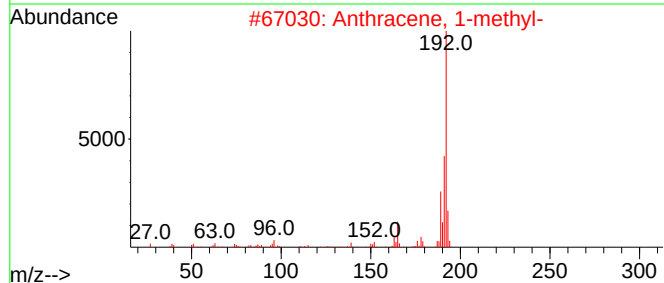
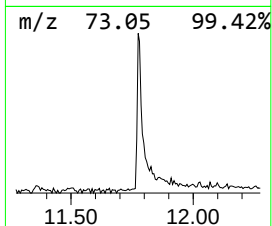
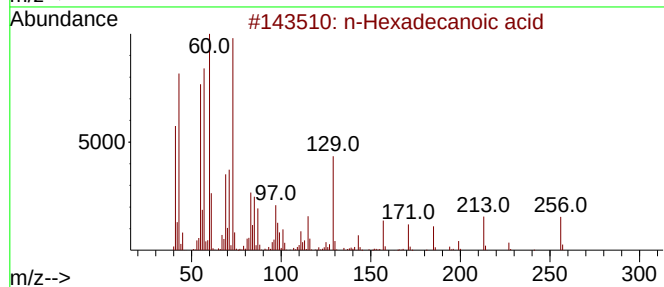
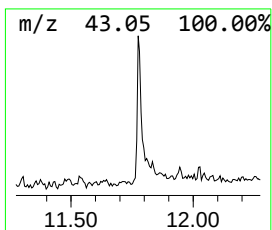
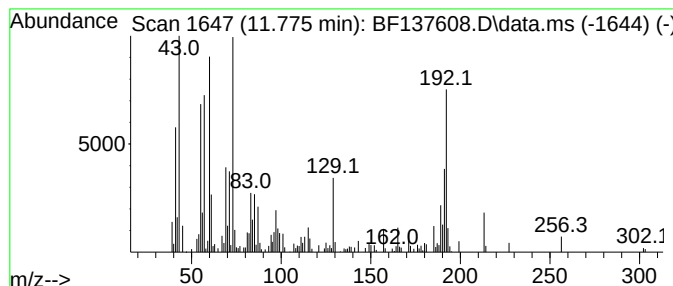
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	3.90 ng	183361	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	55
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55



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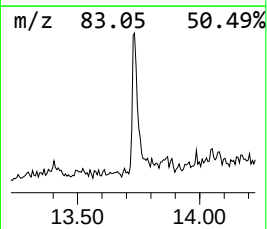
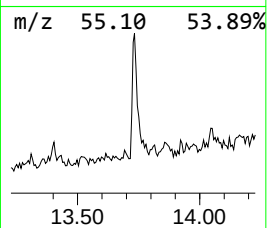
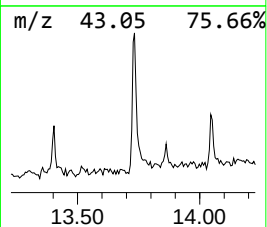
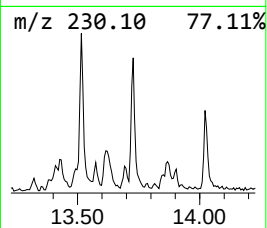
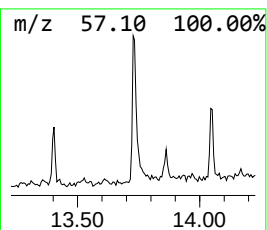
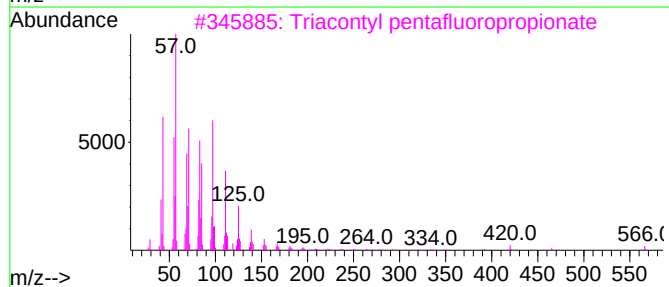
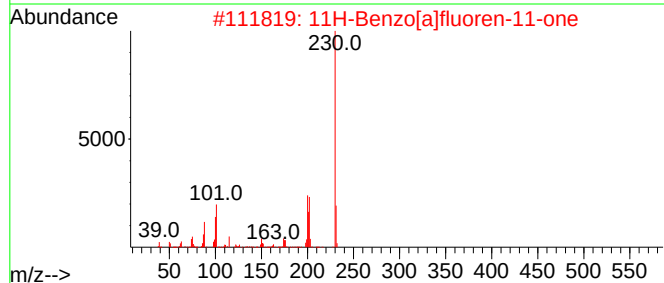
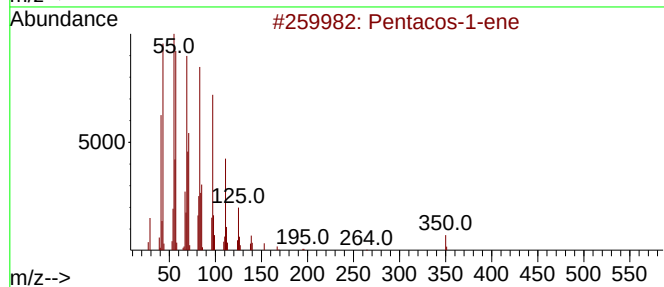
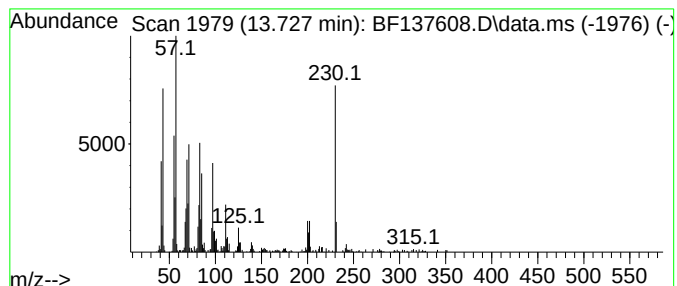
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	3.40 ng	247719	Chrysene-d12	13.874

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacos-1-ene	350	C25H50	016980-85-1	83
2		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	55
3		Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	55
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	55
5		Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	55



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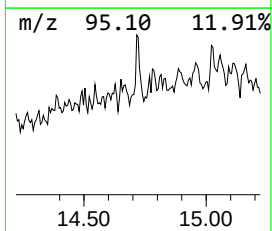
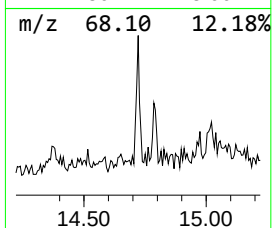
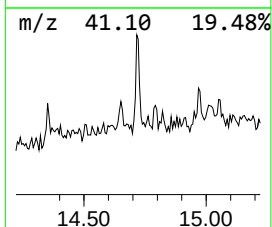
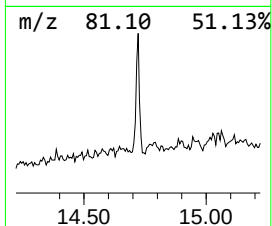
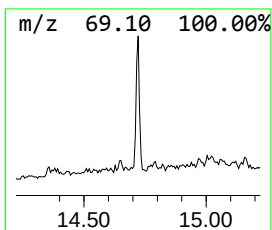
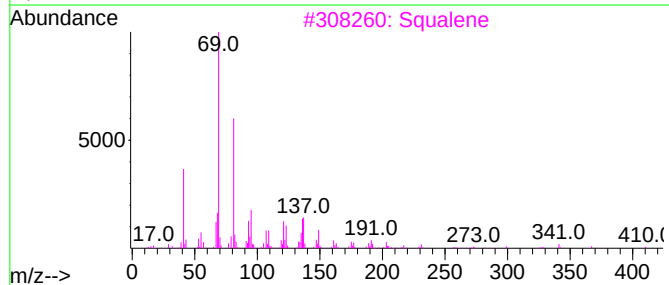
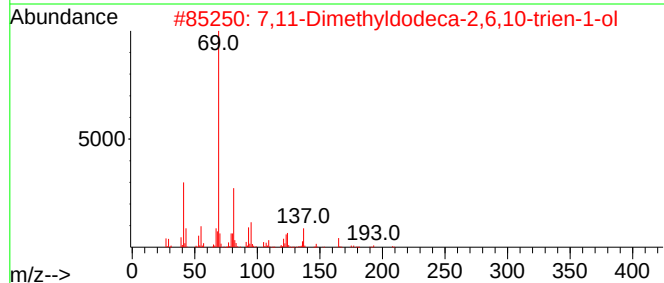
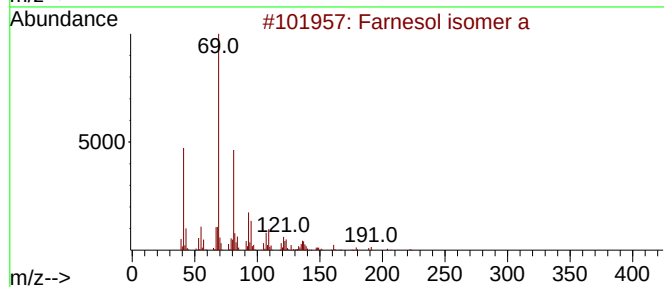
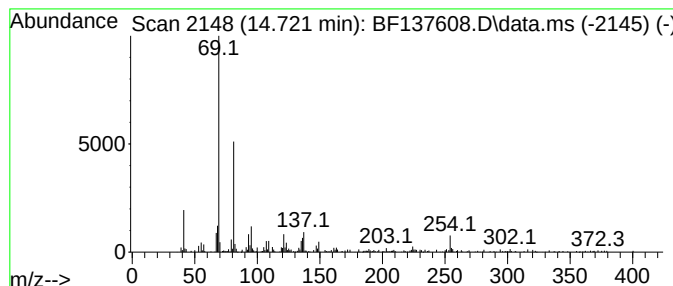
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Farnesol isomer a Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.68 ng	109728	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	72
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			Squalene	410	C30H50	000111-02-4	72
4			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64



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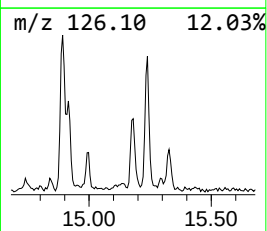
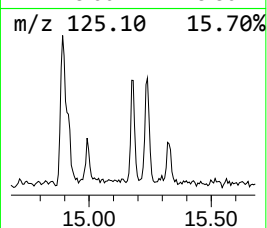
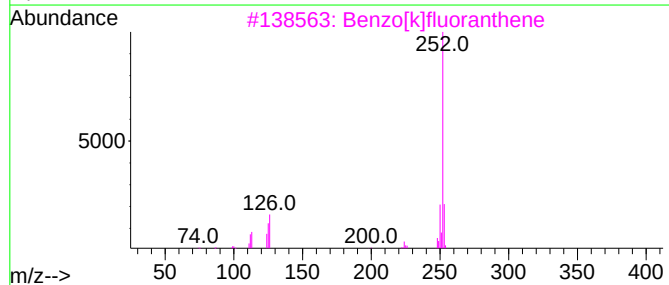
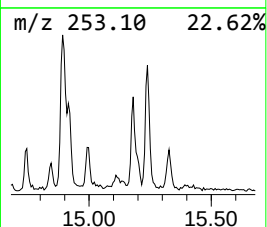
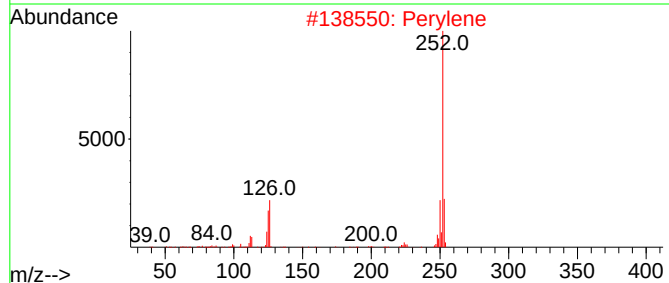
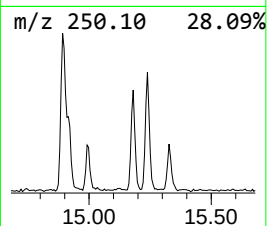
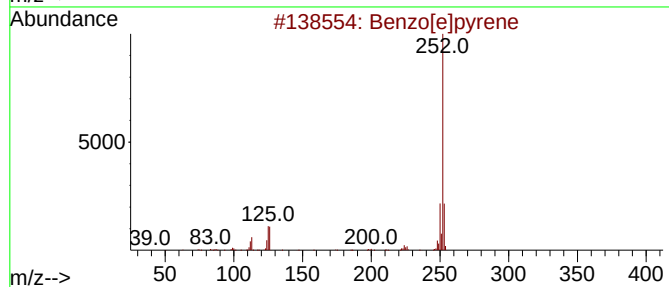
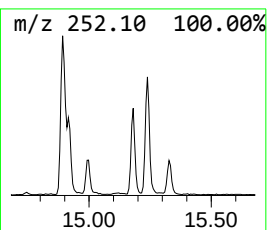
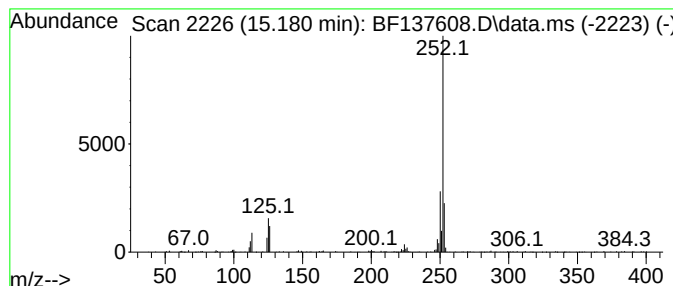
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	5.11 ng	209607	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.775	3.9	ng	183361	4	11.239	939751	20.0
Pentacos-1-ene	13.727	3.4	ng	247719	5	13.874	1456770	20.0
Farnesol isomer a	14.721	2.7	ng	109728	6	15.298	819889	20.0
Benzo[e]pyrene	15.180	5.1	ng	209607	6	15.298	819889	20.0