

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
 Data File : BF129250.D
 Acq On : 15 Jul 2022 21:30
 Operator : CG\JU
 Sample : N3693-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-230

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-BF071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.140	482	485	495	rVB	95991	118360	1.77%	0.222%
2	5.522	545	550	553	rBV	5979314	5650127	84.48%	10.603%
3	6.522	715	720	723	rBV	5321715	5839852	87.31%	10.959%
4	6.898	780	784	787	rBV	1742616	1542354	23.06%	2.894%
5	7.457	874	879	882	rBV	3728947	3807758	56.93%	7.145%
6	8.181	997	1002	1005	rBV	2287979	2165185	32.37%	4.063%
7	9.257	1179	1185	1188	rBV	6841252	6688408	100.00%	12.551%
8	9.933	1294	1300	1304	rBV	2768300	2423986	36.24%	4.549%
9	9.969	1304	1306	1309	rVB	136877	107312	1.60%	0.201%
10	10.139	1329	1335	1339	rBV	78693	89796	1.34%	0.169%
11	10.480	1390	1393	1398	rVB	126189	102943	1.54%	0.193%
12	10.727	1430	1435	1438	rBV	4416659	4168219	62.32%	7.822%
13	11.421	1549	1553	1556	rBV	2641180	2436393	36.43%	4.572%
14	11.445	1556	1557	1561	rVV	999057	685676	10.25%	1.287%
15	11.498	1561	1566	1569	rVB	121051	130470	1.95%	0.245%
16	11.651	1587	1592	1598	rBV	85317	94519	1.41%	0.177%
17	11.939	1635	1641	1646	rBV2	622902	758178	11.34%	1.423%
18	12.039	1654	1658	1660	rBV2	119544	126326	1.89%	0.237%
19	12.245	1690	1693	1696	rVB	122807	100815	1.51%	0.189%
20	12.639	1756	1760	1763	rBV	974018	884479	13.22%	1.660%
21	12.727	1772	1775	1779	rBV2	93305	94103	1.41%	0.177%
22	12.868	1792	1799	1802	rVB	713035	740423	11.07%	1.389%
23	13.010	1819	1823	1826	rVB	6021816	5759095	86.11%	10.807%
24	13.698	1937	1940	1945	rVB	59006	68242	1.02%	0.128%
25	13.898	1971	1974	1987	rBV2	709442	1061275	15.87%	1.992%
26	14.039	1994	1998	2000	rBV	2109327	1975610	29.54%	3.707%
27	14.068	2000	2003	2005	rVV	1551511	1580688	23.63%	2.966%
28	14.092	2005	2007	2012	rVB	265327	223369	3.34%	0.419%
29	14.162	2014	2019	2025	rBV	373902	456808	6.83%	0.857%
30	14.215	2025	2028	2032	rBV3	57717	67365	1.01%	0.126%
31	14.521	2077	2080	2081	rBV	94642	88238	1.32%	0.166%
32	14.539	2081	2083	2088	rVB3	86273	131520	1.97%	0.247%
33	14.833	2130	2133	2137	rVB	64869	68926	1.03%	0.129%
34	14.910	2143	2146	2150	rBV	256303	269824	4.03%	0.506%
35	14.980	2156	2158	2162	rVB	74034	68210	1.02%	0.128%
36	15.115	2177	2181	2184	rBV	197148	301547	4.51%	0.566%

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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

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37	15.174	2188	2191	2195	rVB	112725	117526	1.76%	0.221%
38	15.221	2196	2199	2204	rVV2	65703	96883	1.45%	0.182%
39	15.427	2230	2234	2240	rVB	117332	158912	2.38%	0.298%
40	15.486	2241	2244	2250	rVB	150077	182703	2.73%	0.343%
41	15.557	2251	2256	2267	rBV2	1115888	1469139	21.97%	2.757%
42	16.009	2329	2333	2339	rVB	112949	162207	2.43%	0.304%
43	17.051	2507	2510	2520	rVB2	57971	109630	1.64%	0.206%
44	17.509	2584	2588	2595	rVB	56623	115867	1.73%	0.217%

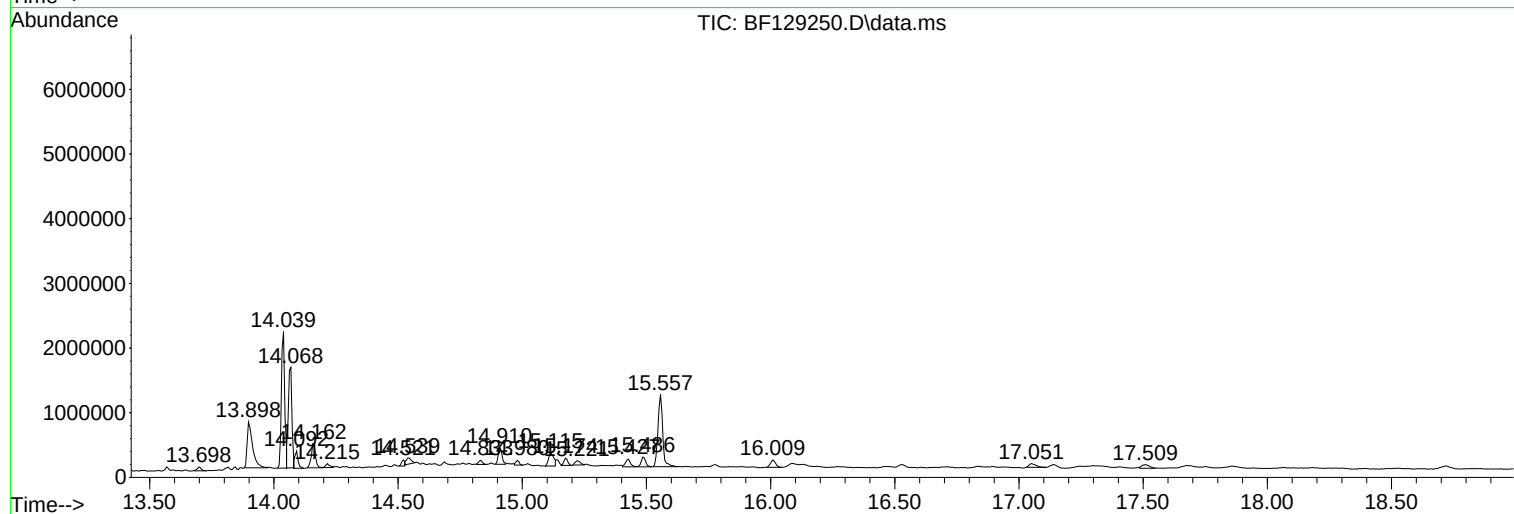
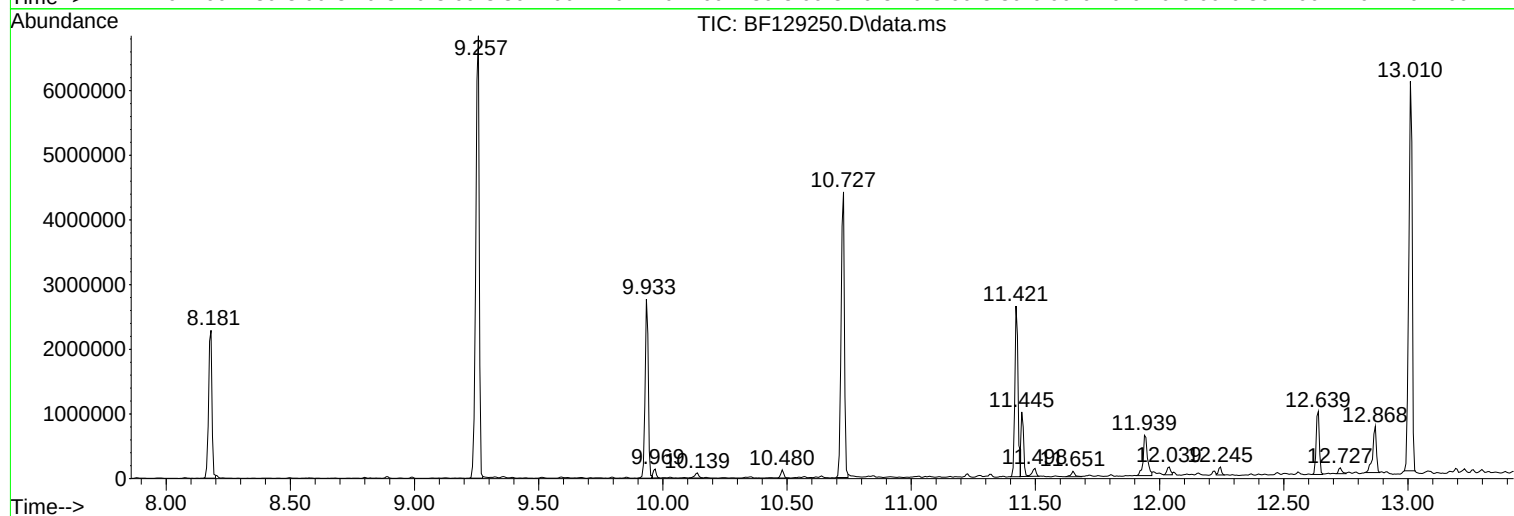
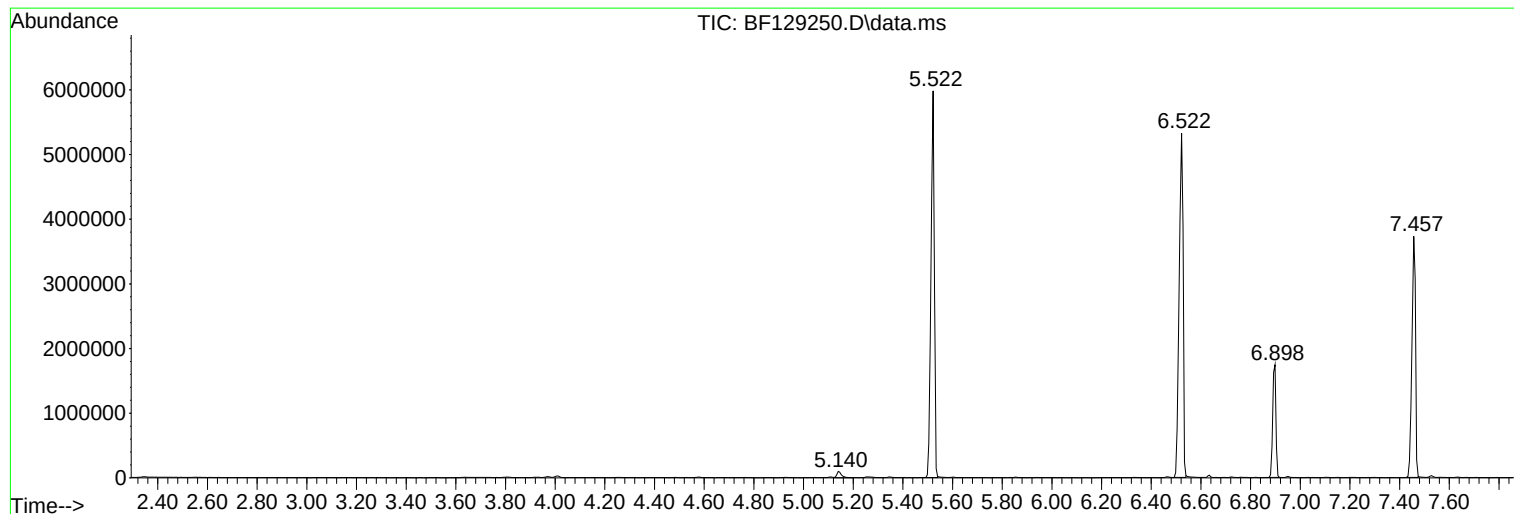
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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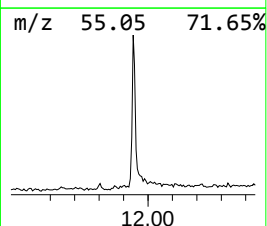
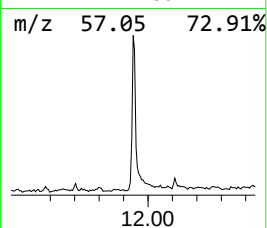
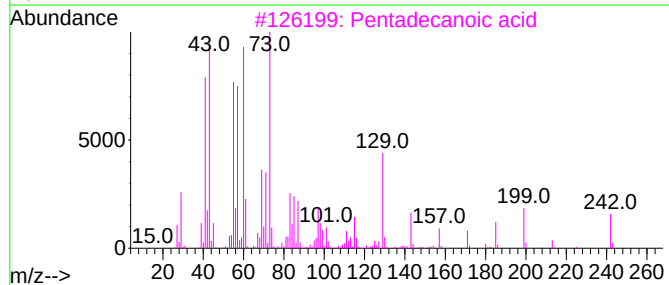
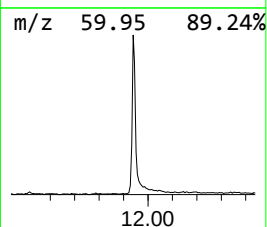
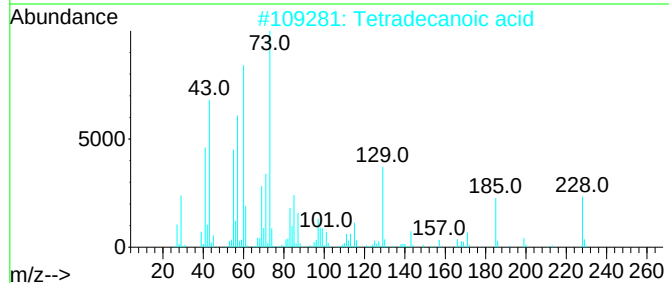
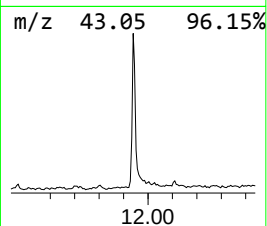
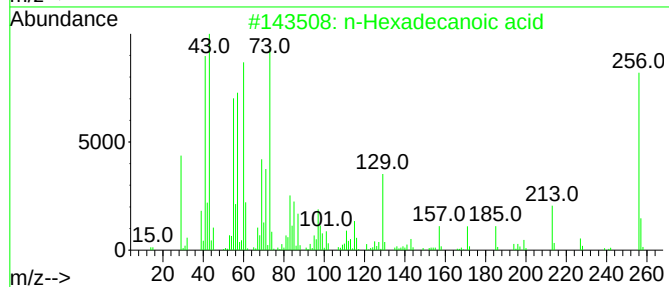
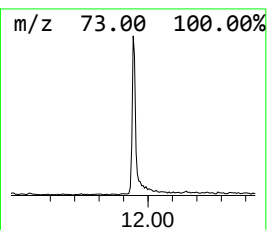
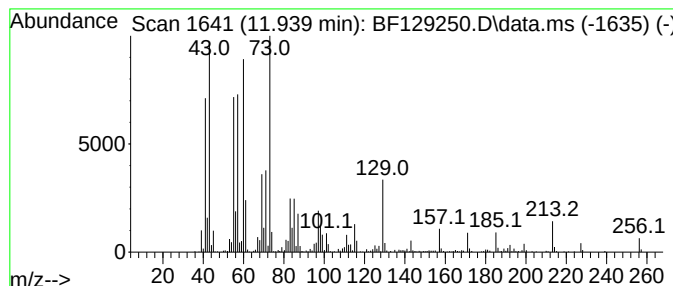
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.939	6.22 ng	758178	Phenanthrene-d10	11.422

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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		Dodecanoic acid	200	C12H24O2	000143-07-7	62



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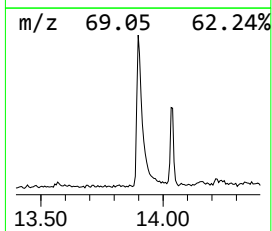
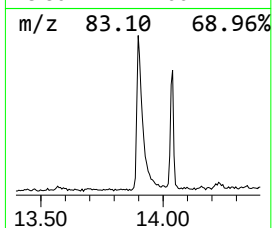
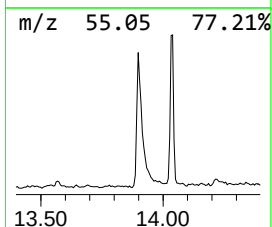
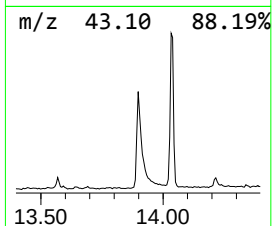
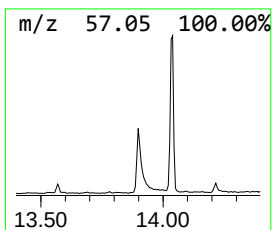
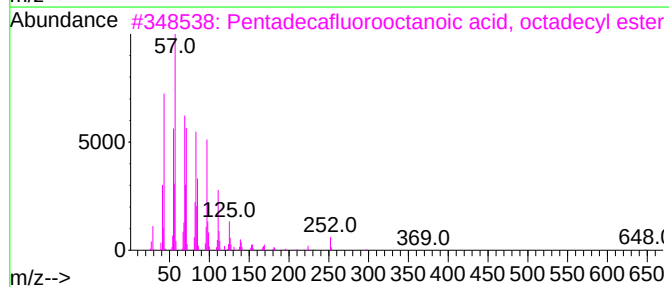
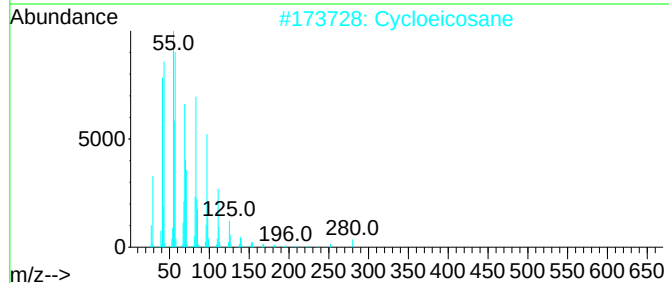
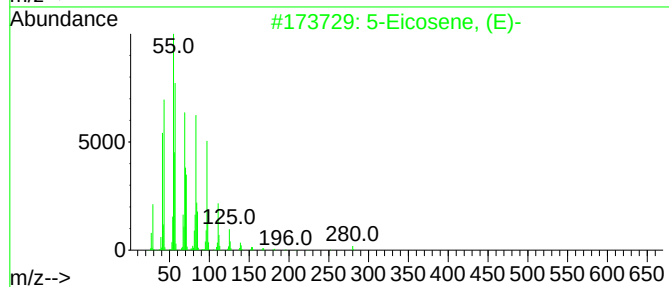
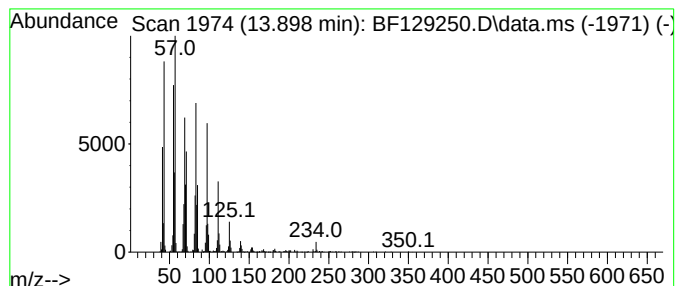
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	13.43 ng	1061280	Chrysene-d12	14.068

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2		Cycloeicosane	280	C20H40	000296-56-0	94
3		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4		1-Hexacosene	364	C26H52	018835-33-1	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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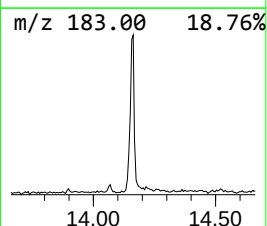
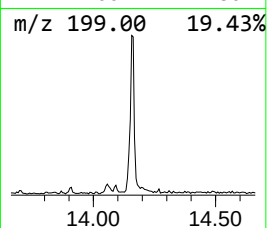
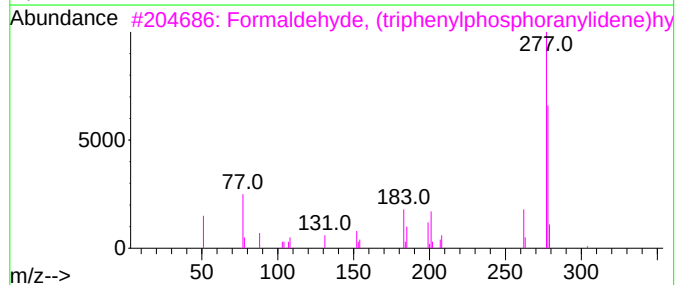
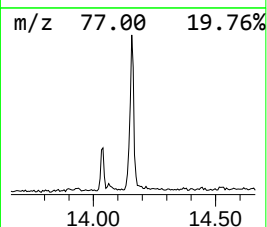
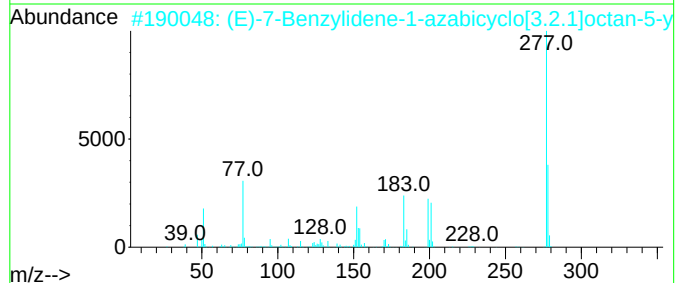
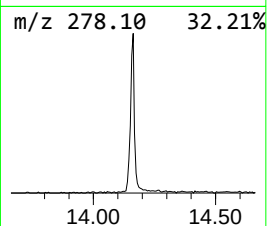
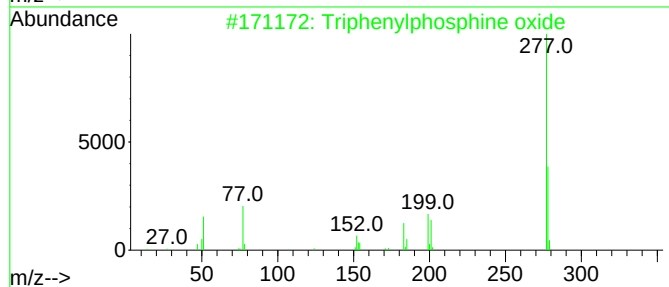
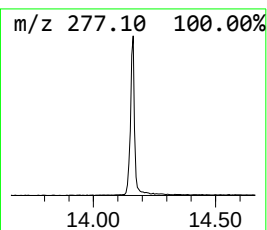
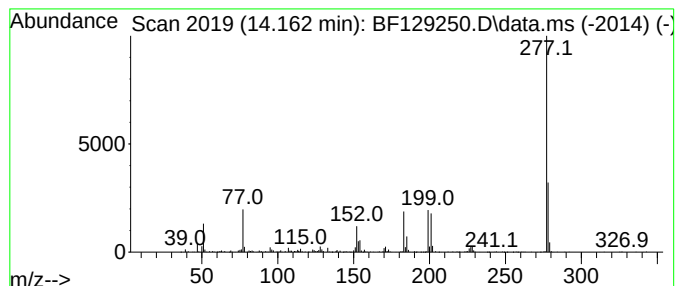
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	5.78 ng	456808	Chrysene-d12	14.068

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	58
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33



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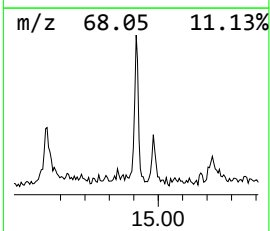
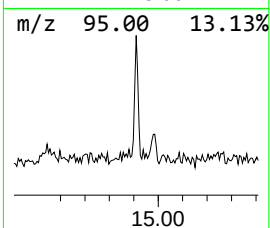
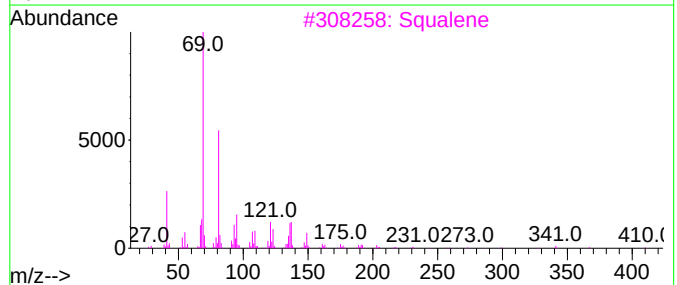
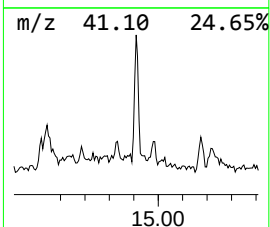
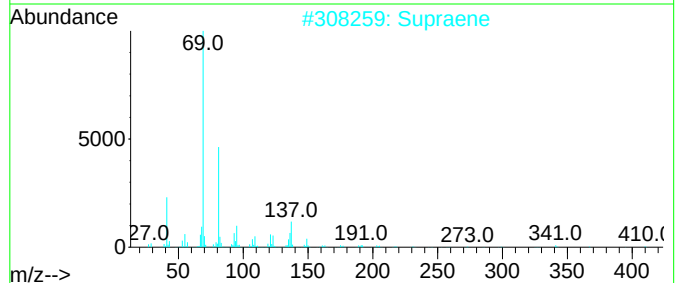
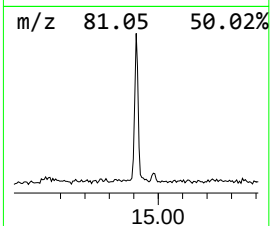
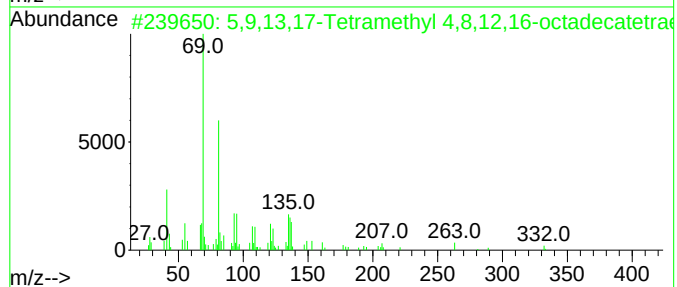
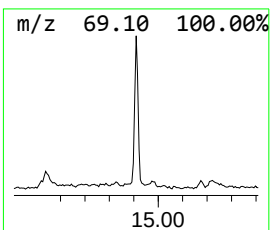
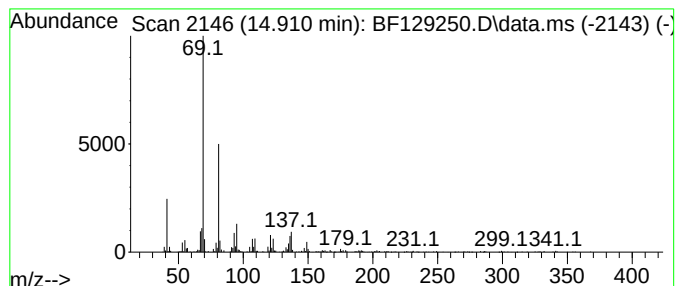
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5,9,13,17-Tetramethyl 4,8,12,16-octadecatetraenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	3.67 ng	269824	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,9,13,17-Tetramethyl 4,8,12,16-octadecatetraenoic acid	332	C22H36O2	1000432-37-9	91		
2	Supraene	410	C30H50	007683-64-9	91		
3	Squalene	410	C30H50	000111-02-4	91		
4	7,11-Dimethyldodeca-2,6,10-trien-5-ol	208	C14H24O	125529-10-4	72		
5	2,6,10,14-Hexadecatetraenoic acid	332	C22H36O2	024035-35-6	72		



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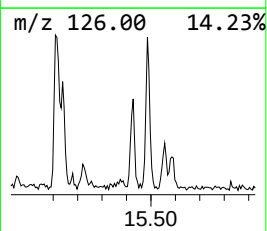
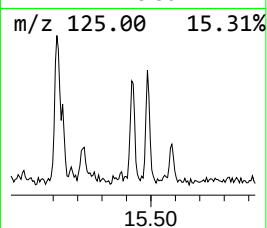
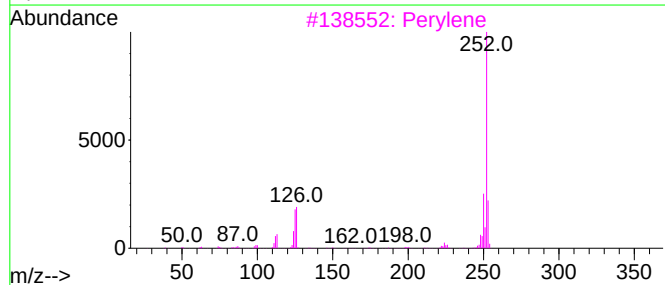
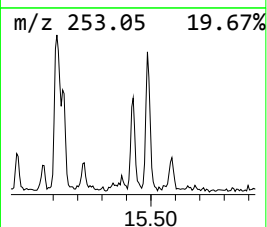
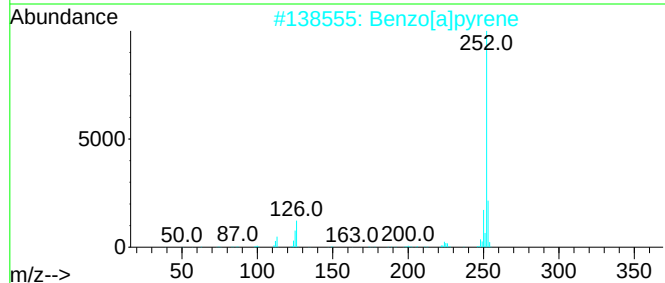
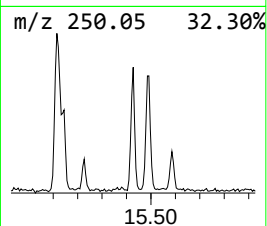
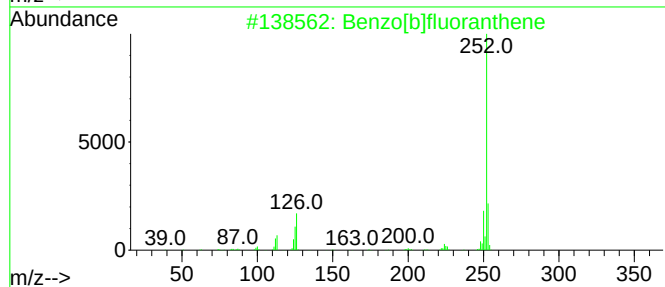
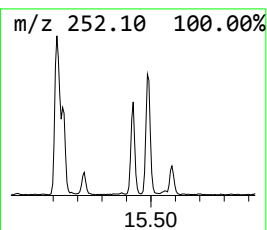
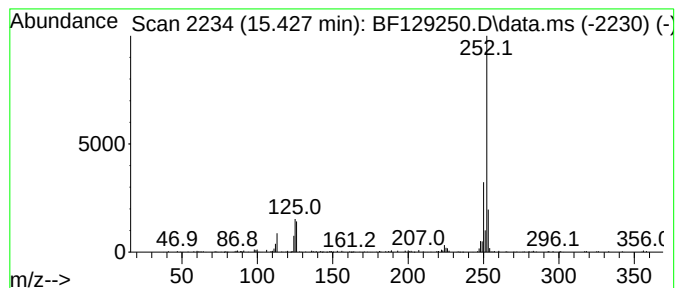
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.16 ng	158912	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	94
3			Perylene	252	C20H12	000198-55-0	94
4			Benzo[e]pyrene	252	C20H12	000192-97-2	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129250.D
Acq On : 15 Jul 2022 21:30
Operator : CG\JU
Sample : N3693-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-230

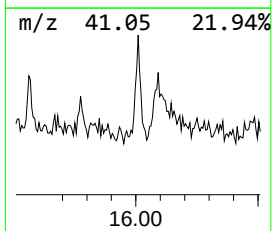
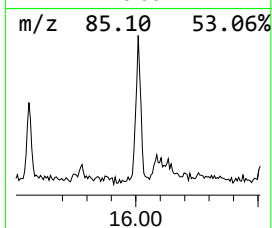
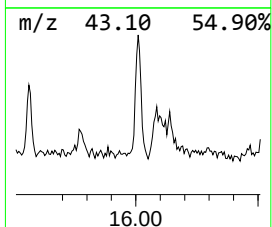
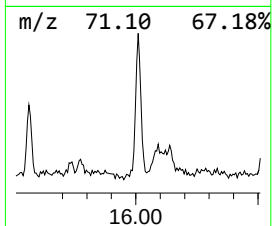
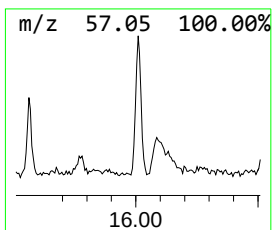
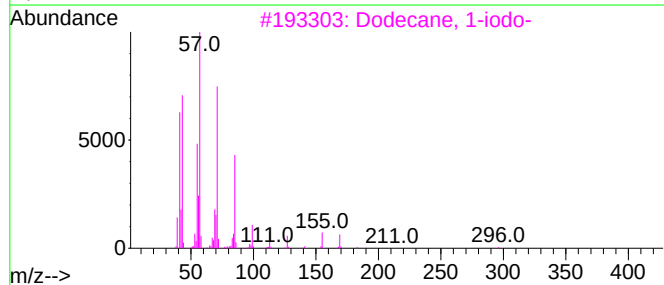
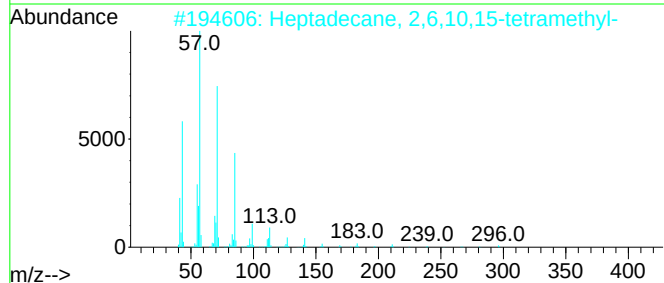
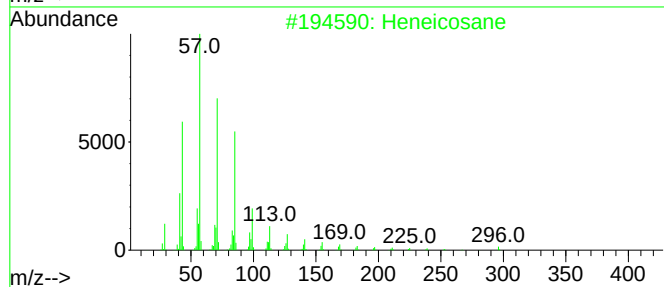
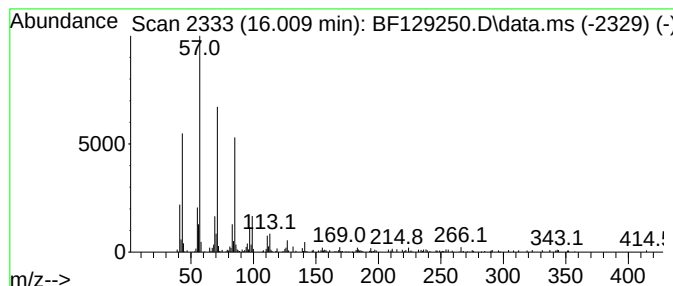
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.21 ng	162207	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
4			Pentacosane	352	C25H52	000629-99-2	78
5			Hexacosane	366	C26H54	000630-01-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129250.D
Acq On : 15 Jul 2022 21:30
Operator : CG\JU
Sample : N3693-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-230

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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
n-Hexadecanoic ...	11.939	6.2	ng	758178	4	11.422	2436390	20.0
5-Eicosene, (E)-	13.898	13.4	ng	1061280	5	14.068	1580690	20.0
Triphenylphosph...	14.163	5.8	ng	456808	5	14.068	1580690	20.0
5,9,13,17-Tetra...	14.910	3.7	ng	269824	6	15.557	1469140	20.0
Perylene	15.427	2.2	ng	158912	6	15.557	1469140	20.0
Heneicosane	16.009	2.2	ng	162207	6	15.557	1469140	20.0