

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042421\
 Data File : BF123722.D
 Acq On : 24 Apr 2021 17:51
 Operator : JU/CG
 Sample : M2107-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-30-9.5-10.0

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123722.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	494	499	505	rBV	62947	85356	1.64%	0.216%
2	5.439	566	570	573	rBV	5003067	4746726	91.42%	12.009%
3	6.451	738	742	750	rBV	5046627	4896161	94.30%	12.387%
4	6.822	801	805	808	rBV	1612729	1385079	26.68%	3.504%
5	7.381	896	900	903	rBV	3737075	3170617	61.06%	8.022%
6	8.104	1019	1023	1026	rBV	2330526	1794143	34.55%	4.539%
7	9.180	1202	1206	1209	rBV	6385810	4972576	95.77%	12.581%
8	9.569	1270	1272	1276	rBV	157420	139399	2.68%	0.353%
9	9.857	1318	1321	1325	rVB	2399896	1943636	37.43%	4.917%
10	10.645	1451	1455	1459	rBV	3791186	3400122	65.48%	8.602%
11	11.345	1570	1574	1577	rBV	2582745	2075971	39.98%	5.252%
12	11.416	1580	1586	1591	rVB6	56339	77920	1.50%	0.197%
13	11.880	1662	1665	1673	rBV	154684	175587	3.38%	0.444%
14	12.933	1840	1844	1847	rBV	5823339	5192384	100.00%	13.137%
15	13.474	1931	1936	1940	rBV3	56697	67897	1.31%	0.172%
16	13.851	1993	2000	2015	rBV2	253296	803331	15.47%	2.032%
17	13.986	2017	2023	2026	rVV	2182381	2010437	38.72%	5.086%
18	14.009	2026	2027	2036	rVB	54157	64336	1.24%	0.163%
19	14.462	2099	2104	2108	rBV	96499	108041	2.08%	0.273%
20	14.768	2150	2156	2161	rVB	82466	99353	1.91%	0.251%
21	14.845	2165	2169	2172	rBV	251770	228565	4.40%	0.578%
22	15.104	2210	2213	2220	rBV	111273	128765	2.48%	0.326%
23	15.227	2230	2234	2247	rVB	52308	163093	3.14%	0.413%
24	15.451	2266	2272	2276	rBV	1129057	1406077	27.08%	3.557%
25	15.486	2276	2278	2283	rVB	98740	99767	1.92%	0.252%
26	15.915	2347	2351	2358	rVB	83231	128467	2.47%	0.325%
27	16.421	2433	2437	2441	rVB2	55148	76713	1.48%	0.194%
28	17.015	2532	2538	2545	rVB7	39988	84860	1.63%	0.215%

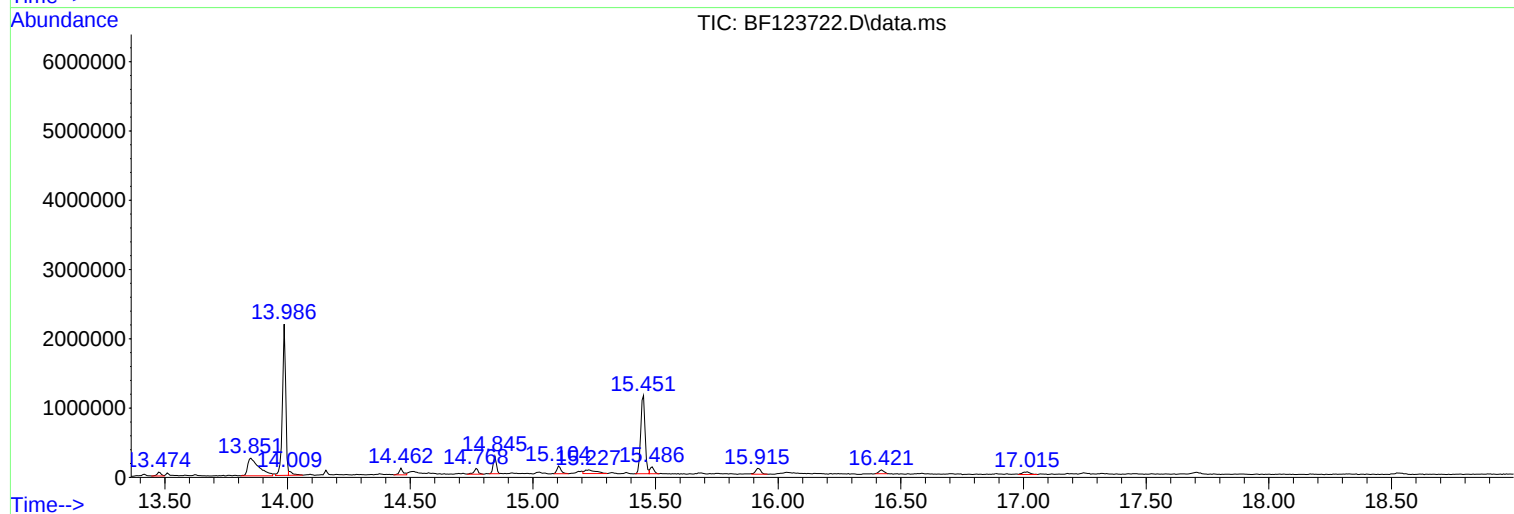
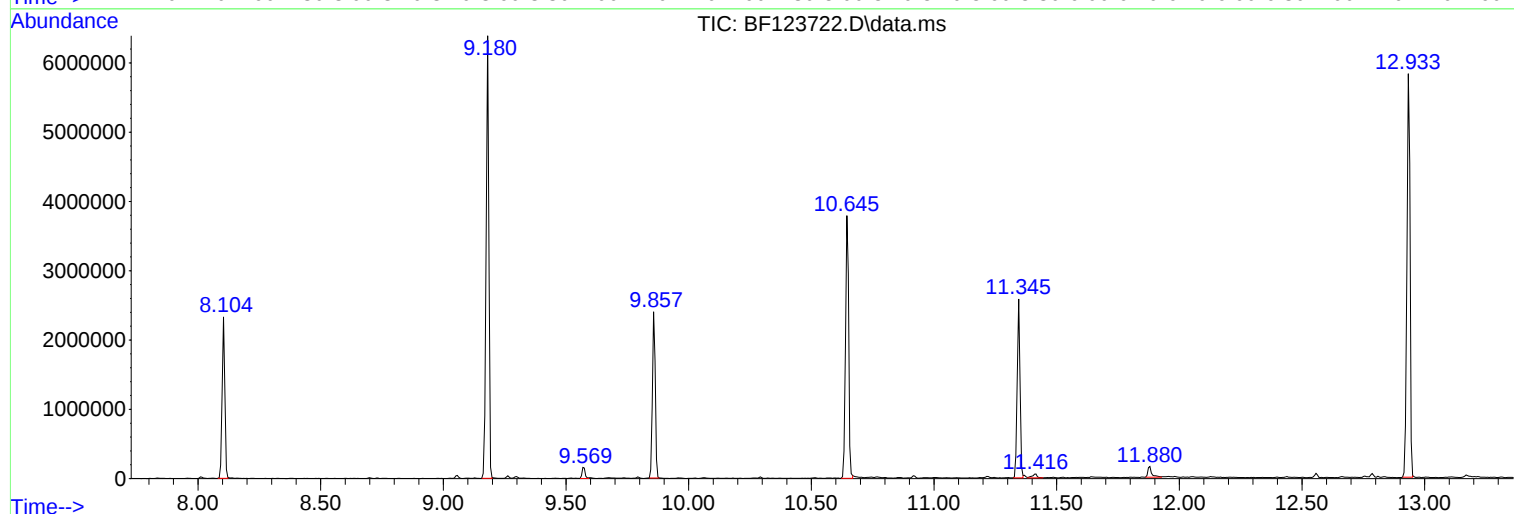
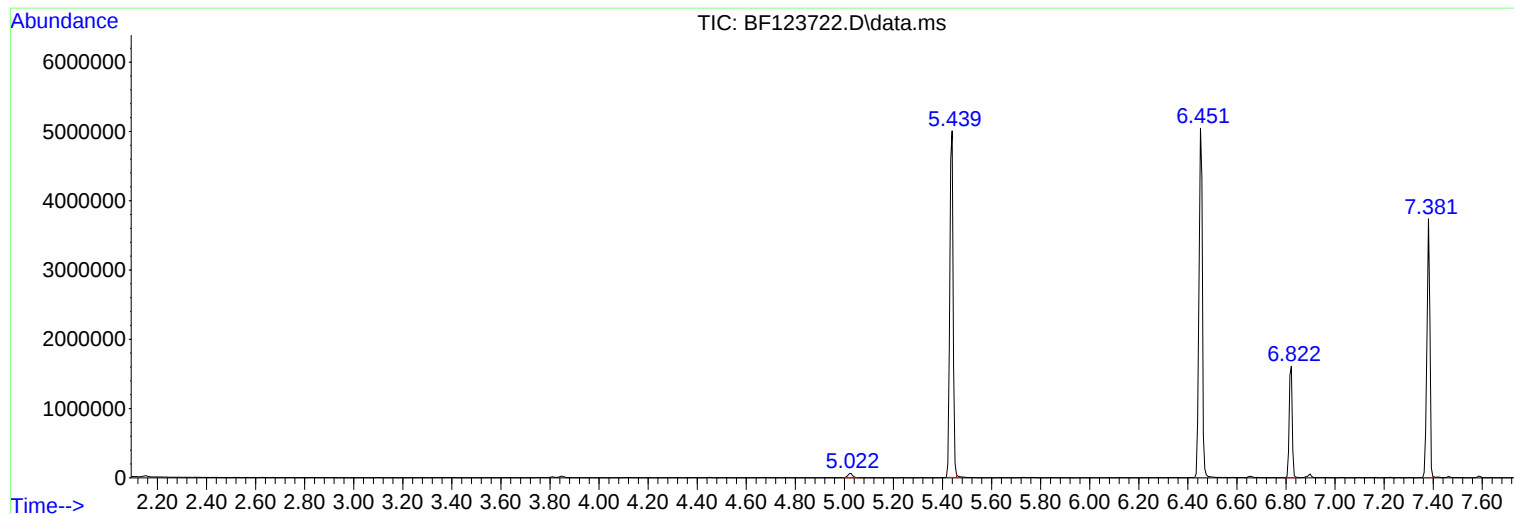
Sum of corrected areas: 39525379

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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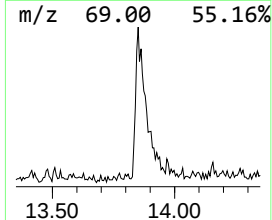
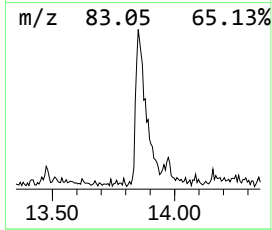
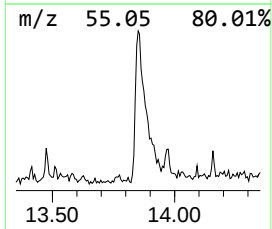
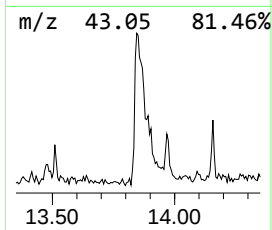
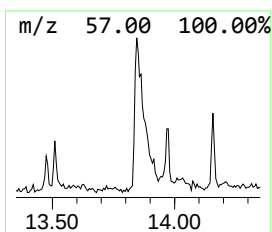
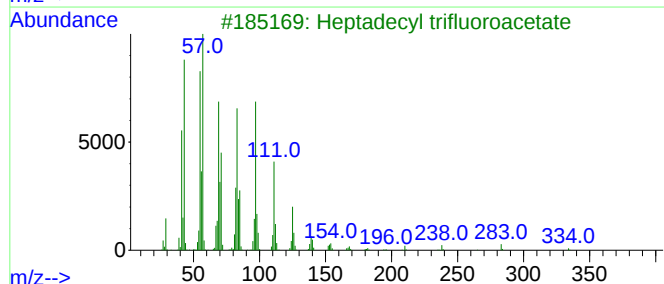
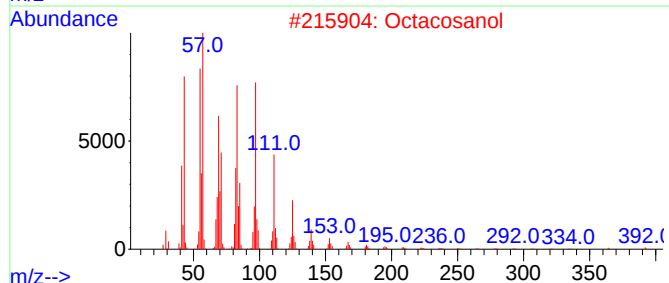
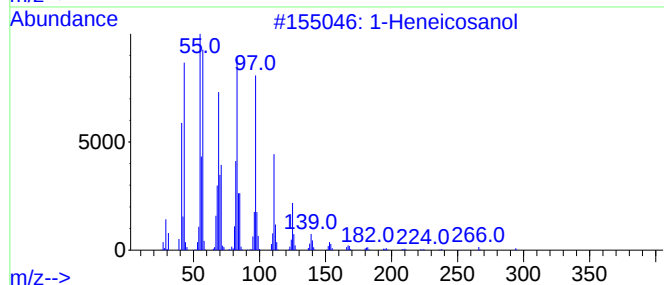
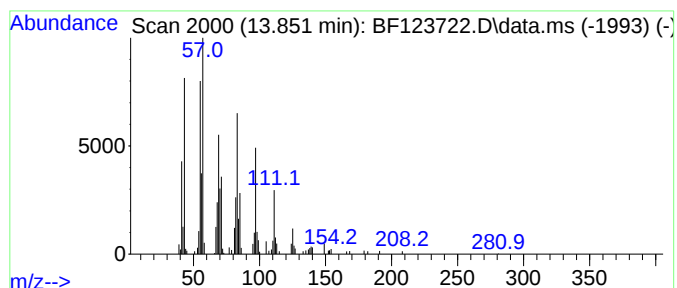
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	7.99 ng	803331	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			Octacosanol	410	C28H58O	000557-61-9	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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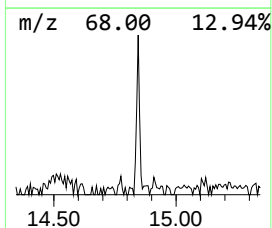
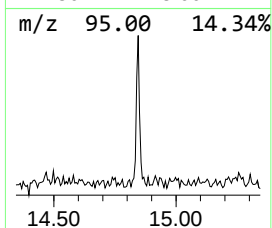
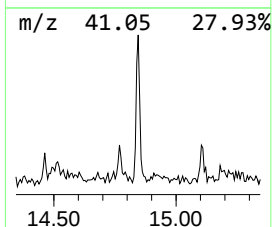
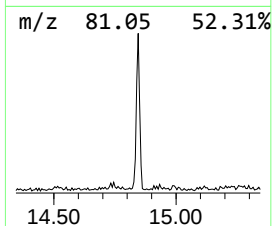
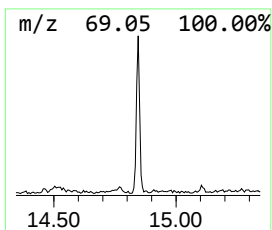
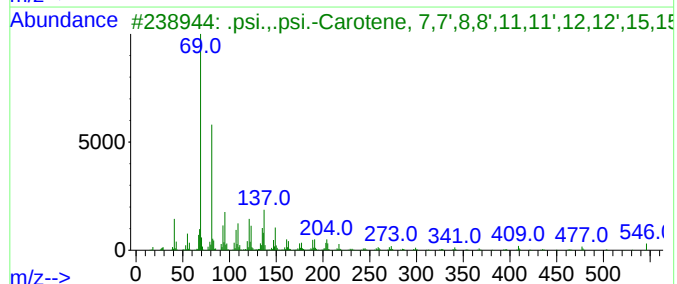
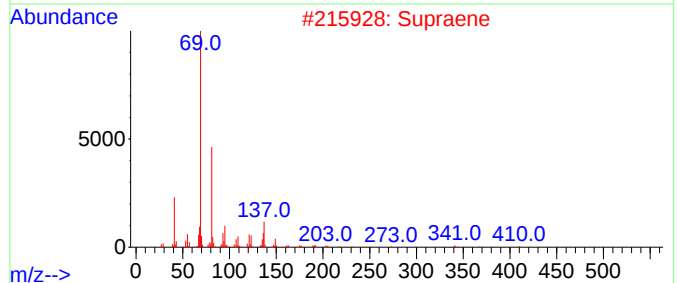
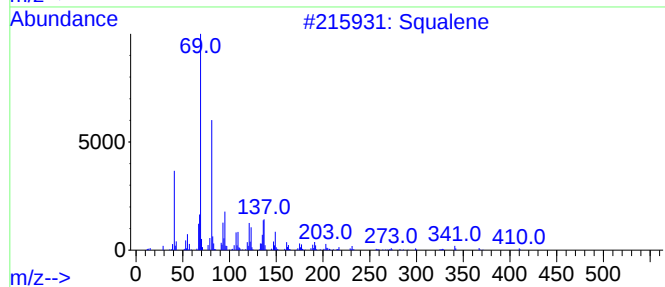
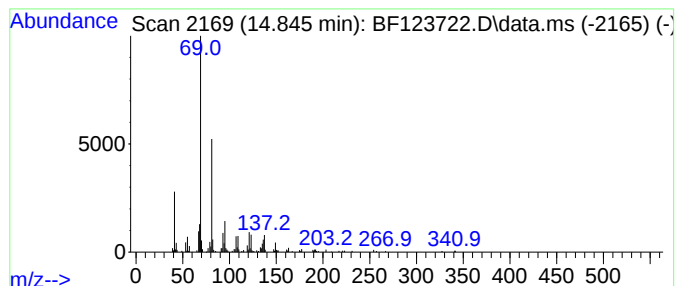
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Peak Number 2 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	3.25 ng	228565	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	87
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72



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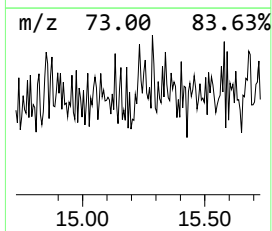
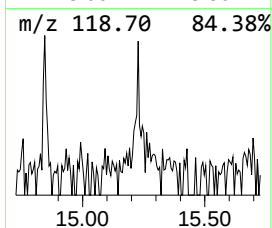
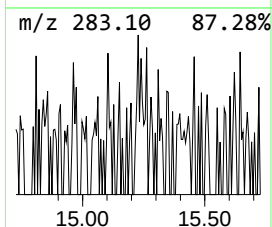
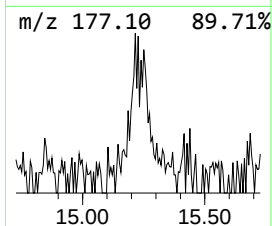
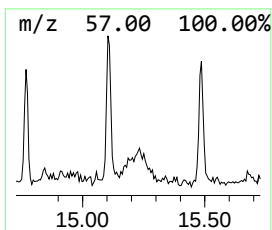
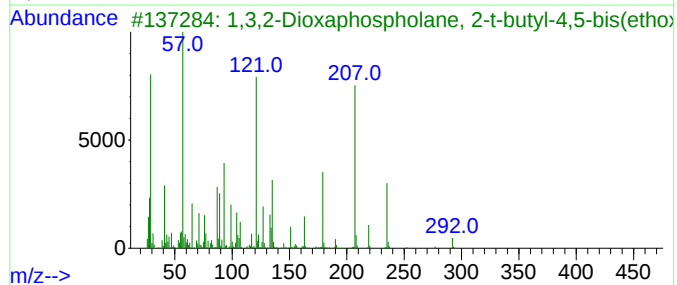
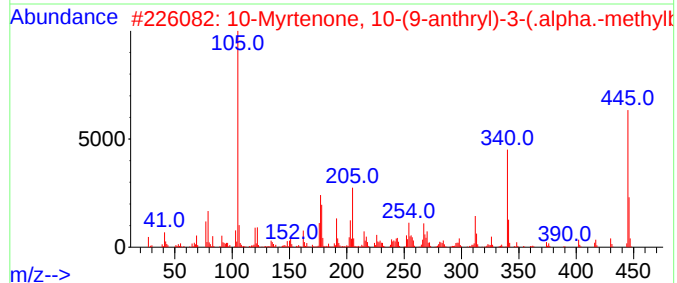
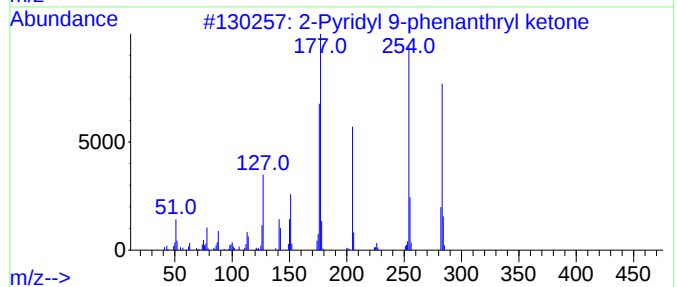
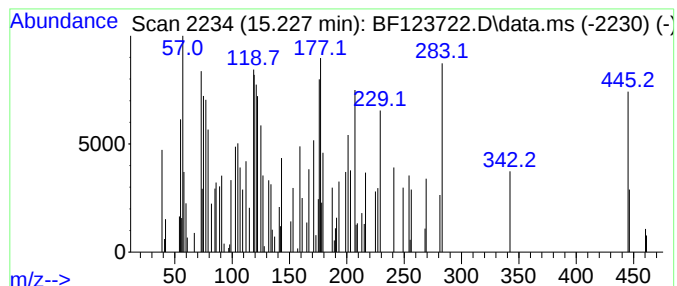
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.227 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	2.32 ng	163093	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyridyl	9-phenanthryl	ketone	283	C20H13NO	056988-72-8	12
2	10-Myrtenone,	10-(9-anthryl)-3-(...		445	C32H31NO	1000163-82-1	10
3	1,3,2-Dioxaphospholane,	2-t-buty...		292	C12H21O6P	080043-97-6	10
4	N-Methyl	nicotinimide,	0-trime...	208	C10H16N2OSi	1000141-33-7	10
5	1H-1,4-Diazepine,	hexahydro-1-(2...		177	C10H15N3	1000337-93-1	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Heneicosanol	13.851	8.0	ng	803331	5	13.986	2010440	20.0
Squalene	14.845	3.3	ng	228565	6	15.451	1406080	20.0
unknown15.227	15.227	2.3	ng	163093	6	15.451	1406080	20.0