

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042421\
 Data File : BF123721.D
 Acq On : 24 Apr 2021 17:19
 Operator : JU/CG
 Sample : M2107-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

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

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: BF123721.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	rVB	117214	149159	2.89%	0.369%
2	5.440	566	570	573	rBV	5064623	4910030	95.13%	12.131%
3	6.451	738	742	749	rBV	5192927	5100887	98.83%	12.603%
4	6.822	801	805	808	rBV	1587320	1384795	26.83%	3.421%
5	7.381	895	900	903	rBV	3874503	3310723	64.14%	8.180%
6	8.104	1019	1023	1026	rBV	2320842	1815237	35.17%	4.485%
7	9.180	1202	1206	1209	rBV	6418232	5039493	97.64%	12.451%
8	9.575	1269	1273	1276	rBV	186164	155865	3.02%	0.385%
9	9.857	1318	1321	1325	rVB	2328610	1933515	37.46%	4.777%
10	9.951	1333	1337	1343	rVB3	85873	84299	1.63%	0.208%
11	10.645	1451	1455	1459	rBV	4075148	3509044	67.98%	8.670%
12	11.345	1570	1574	1577	rBV	2586969	2092235	40.54%	5.169%
13	11.410	1579	1585	1588	rVV4	72440	85331	1.65%	0.211%
14	11.874	1661	1664	1668	rBV	84690	84216	1.63%	0.208%
15	12.833	1825	1827	1830	rVB	93353	66345	1.29%	0.164%
16	12.933	1840	1844	1847	rBV	5583370	5161532	100.00%	12.753%
17	13.168	1881	1884	1886	rBV	88085	71435	1.38%	0.176%
18	13.398	1918	1923	1924	rBV3	73794	71323	1.38%	0.176%
19	13.415	1924	1926	1932	rVB2	62953	62790	1.22%	0.155%
20	13.474	1932	1936	1940	rBV4	69564	99510	1.93%	0.246%
21	13.510	1940	1942	1944	rVB	110013	78739	1.53%	0.195%
22	13.845	1995	1999	2018	rBV2	296369	768318	14.89%	1.898%
23	13.986	2019	2023	2027	rVB	2127529	1874143	36.31%	4.630%
24	14.157	2049	2052	2055	rBV	159261	127435	2.47%	0.315%
25	14.462	2100	2104	2108	rBV	168859	150820	2.92%	0.373%
26	14.768	2153	2156	2160	rVB	130314	117076	2.27%	0.289%
27	14.845	2165	2169	2172	rBV	273110	259225	5.02%	0.640%
28	15.104	2209	2213	2217	rBV	122618	141637	2.74%	0.350%
29	15.445	2266	2271	2275	rBV2	1131524	1467631	28.43%	3.626%
30	15.486	2275	2278	2282	rVB	85575	101979	1.98%	0.252%
31	15.915	2347	2351	2356	rVB2	65939	90942	1.76%	0.225%
32	16.415	2431	2436	2443	rBV3	53843	108365	2.10%	0.268%

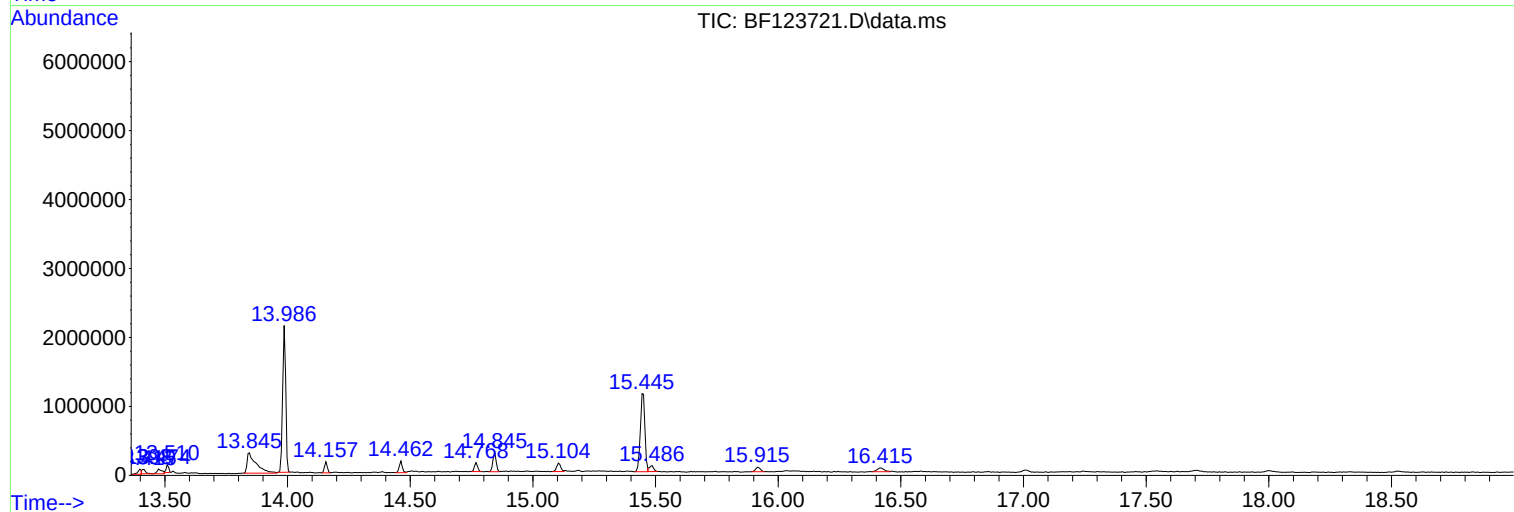
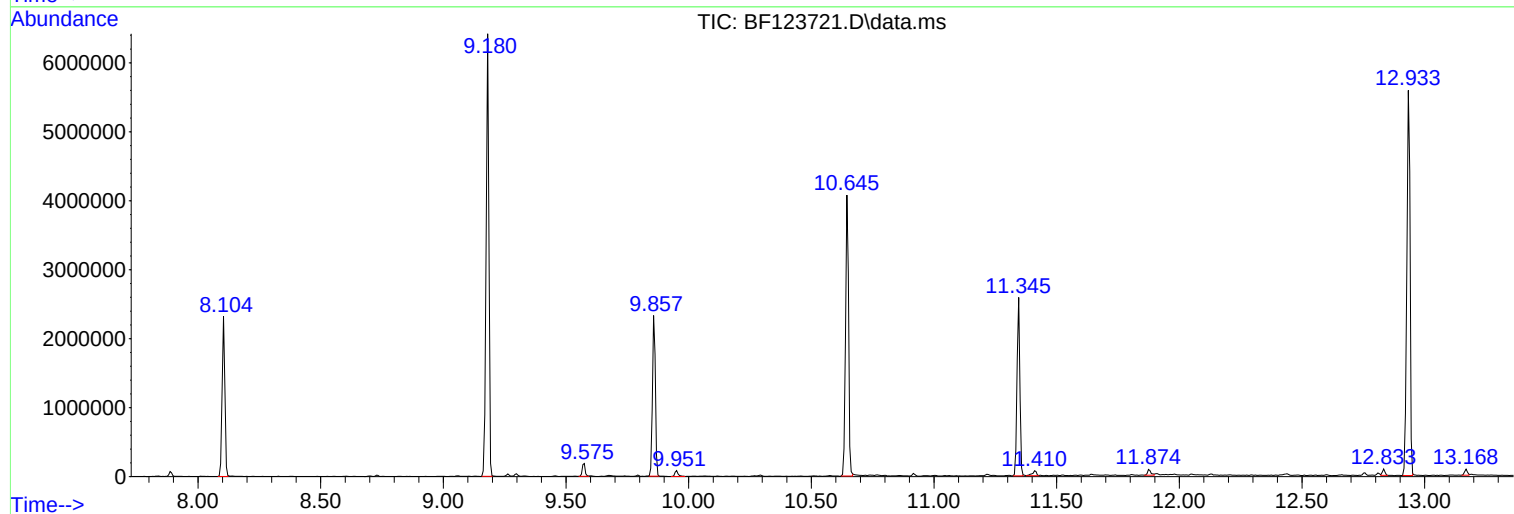
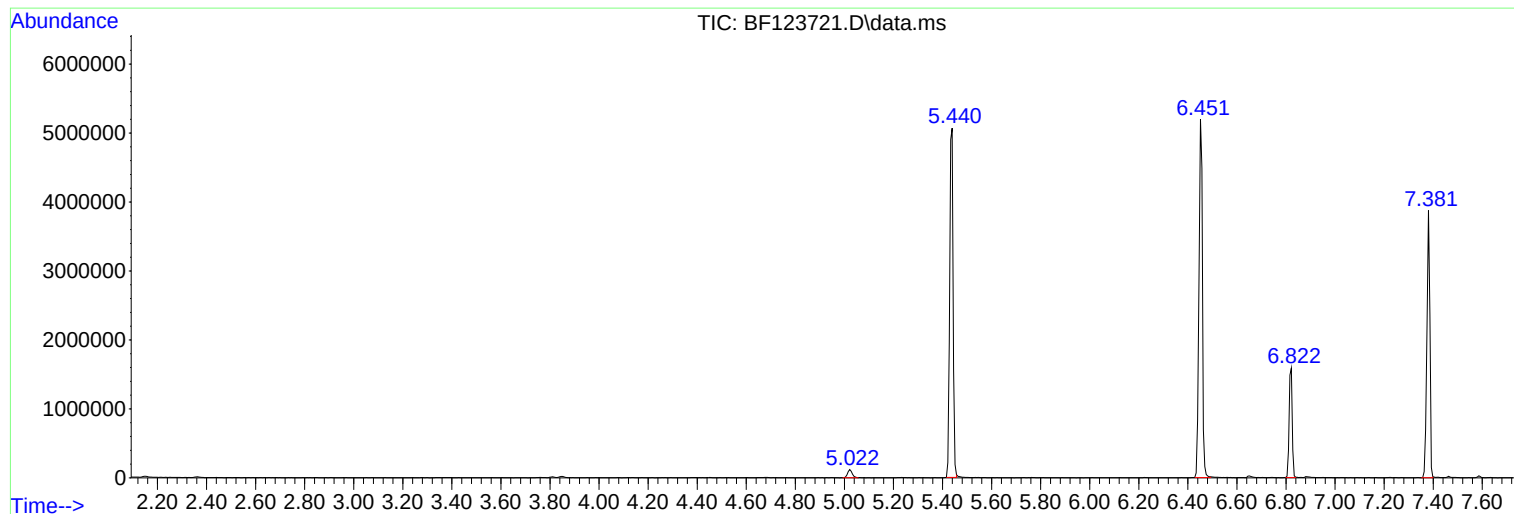
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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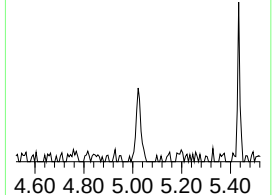
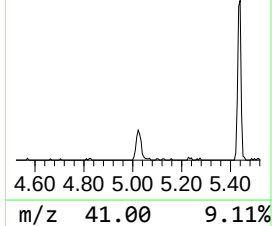
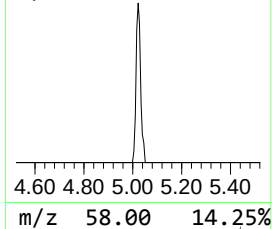
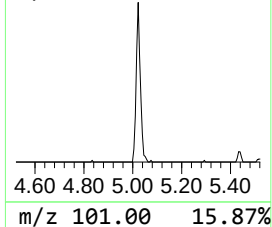
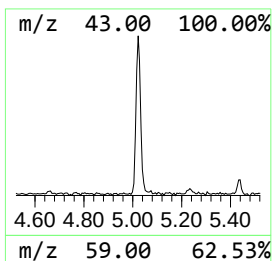
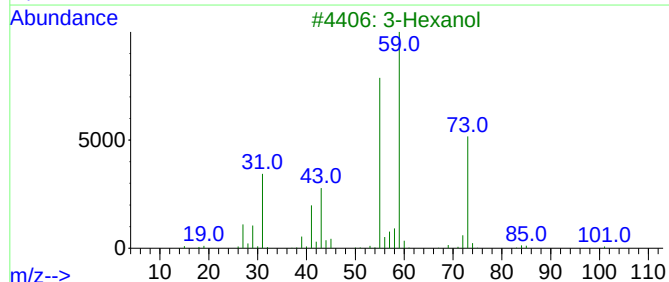
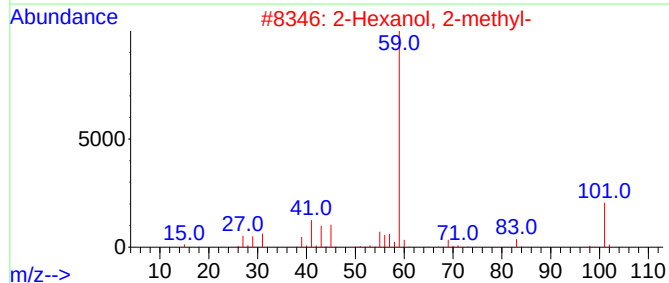
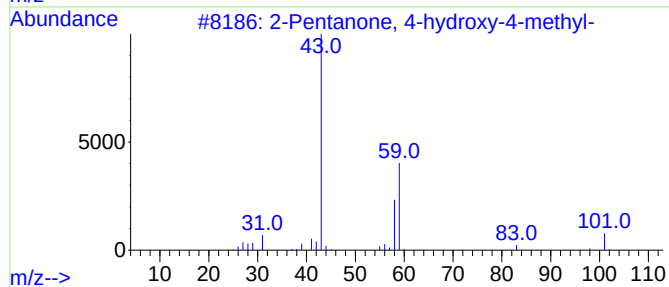
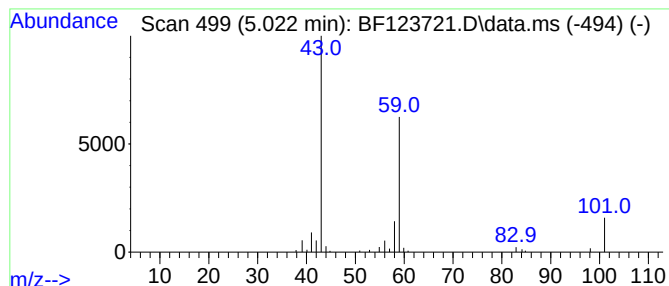
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.15 ng	149159	1,4-Dichlorobenzene-d4	6.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		3-Hexanol	102	C6H14O	000623-37-0	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



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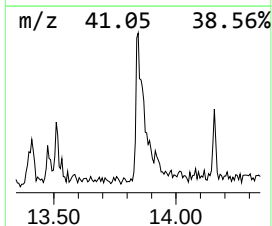
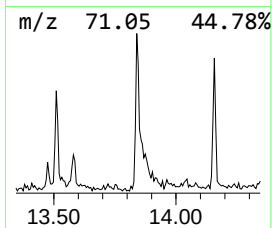
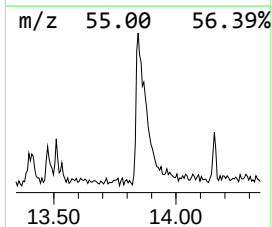
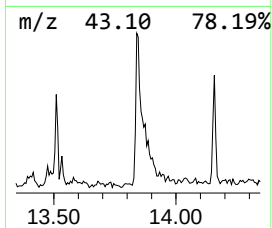
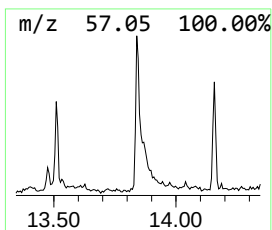
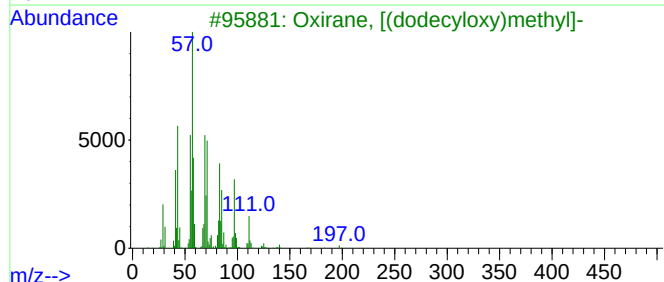
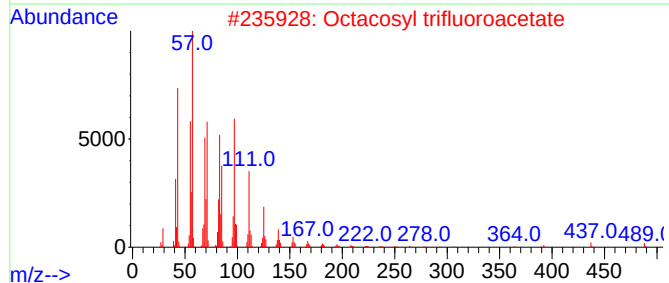
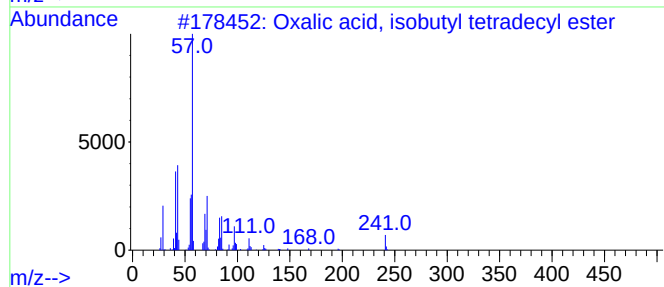
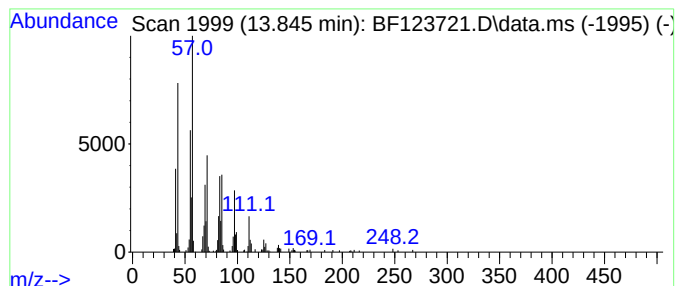
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Peak Number 2 Oxalic acid, isobutyl tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	8.20 ng	768318	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	90
4			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	90
5			Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	83



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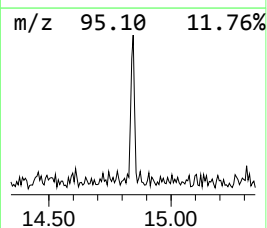
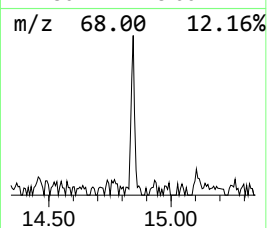
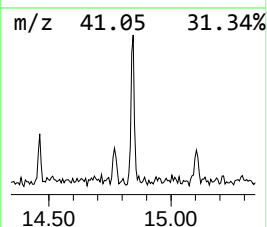
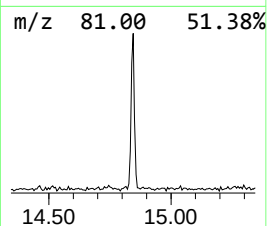
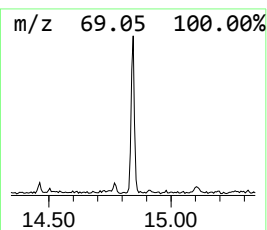
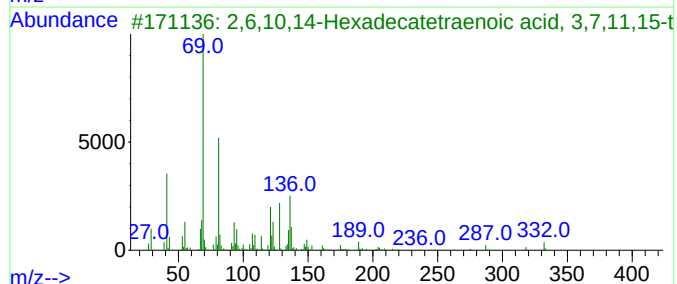
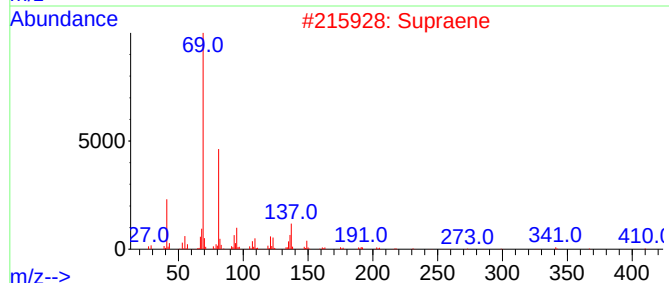
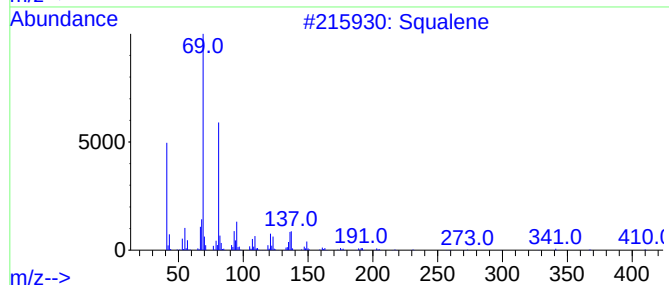
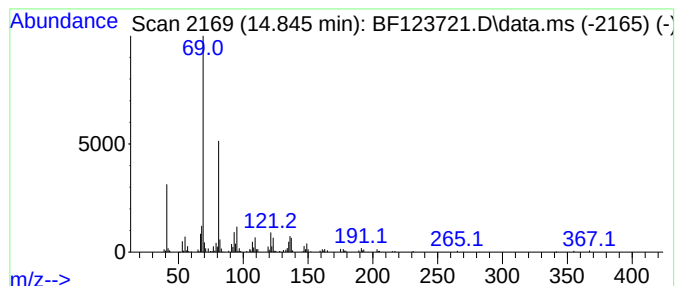
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Peak Number 3 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	3.53 ng	259225	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	83
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5			1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	2.1	ng	149159	1	6.822	1384800	20.0
Oxalic acid, is...	13.845	8.2	ng	768318	5	13.986	1874140	20.0
Squalene	14.845	3.5	ng	259225	6	15.445	1467630	20.0