

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042421\
 Data File : BF123716.D
 Acq On : 24 Apr 2021 14:42
 Operator : JU/CG
 Sample : M2149-15
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-40-9.5-10.0

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: BF123716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	493	500	507	rBV	290058	375102	5.67%	0.803%
2	5.440	566	570	574	rBV	6329140	5865438	88.64%	12.554%
3	6.457	738	743	749	rBV	6634566	6616979	100.00%	14.163%
4	6.822	801	805	808	rBV	1469404	1268363	19.17%	2.715%
5	7.381	895	900	903	rBV	4518489	4621488	69.84%	9.892%
6	8.104	1019	1023	1026	rBV	2096695	1634173	24.70%	3.498%
7	9.180	1201	1206	1209	rBV	7596837	6518895	98.52%	13.953%
8	9.263	1214	1220	1224	rBV	66093	74797	1.13%	0.160%
9	9.569	1269	1272	1276	rBV	226011	189996	2.87%	0.407%
10	9.857	1317	1321	1324	rBV	2178856	1729421	26.14%	3.702%
11	10.645	1451	1455	1459	rBV	4489821	4219755	63.77%	9.032%
12	11.198	1545	1549	1555	rBV3	55632	73837	1.12%	0.158%
13	11.345	1570	1574	1577	rBV	2242494	1801179	27.22%	3.855%
14	12.933	1839	1844	1848	rBV	6190110	6150285	92.95%	13.164%
15	13.168	1881	1884	1889	rBV2	69746	97900	1.48%	0.210%
16	13.474	1933	1936	1940	rBV2	191117	185964	2.81%	0.398%
17	13.692	1970	1973	1978	rVB	100463	90774	1.37%	0.194%
18	13.839	1994	1998	2017	rBV	500503	1325942	20.04%	2.838%
19	13.986	2019	2023	2027	rVB	1658682	1435193	21.69%	3.072%
20	14.462	2101	2104	2105	rBV	136299	115102	1.74%	0.246%
21	14.492	2105	2109	2123	rVB4	225636	610510	9.23%	1.307%
22	14.768	2153	2156	2159	rVB	90415	79851	1.21%	0.171%
23	15.104	2209	2213	2218	rBV	140907	179151	2.71%	0.383%
24	15.445	2266	2271	2275	rBV	924751	1092936	16.52%	2.339%
25	15.486	2275	2278	2282	rVB2	76506	96295	1.46%	0.206%
26	15.915	2347	2351	2355	rBV3	64103	97506	1.47%	0.209%
27	16.421	2433	2437	2444	rVB3	51072	89772	1.36%	0.192%
28	17.074	2544	2548	2555	rBV10	42847	83535	1.26%	0.179%

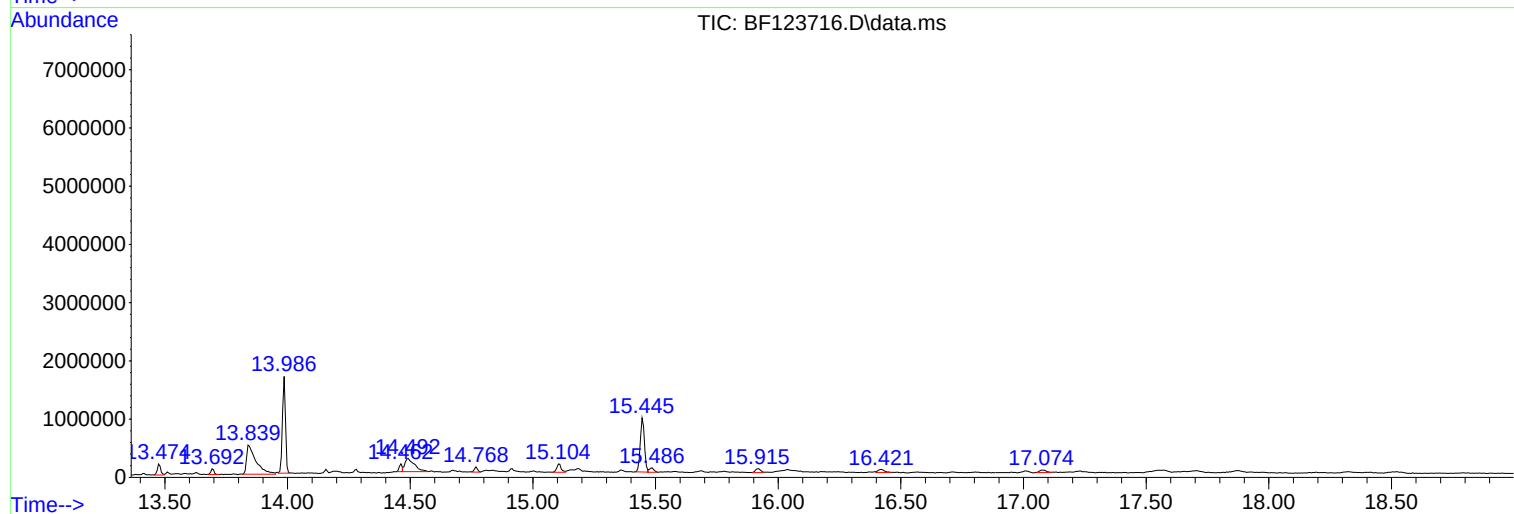
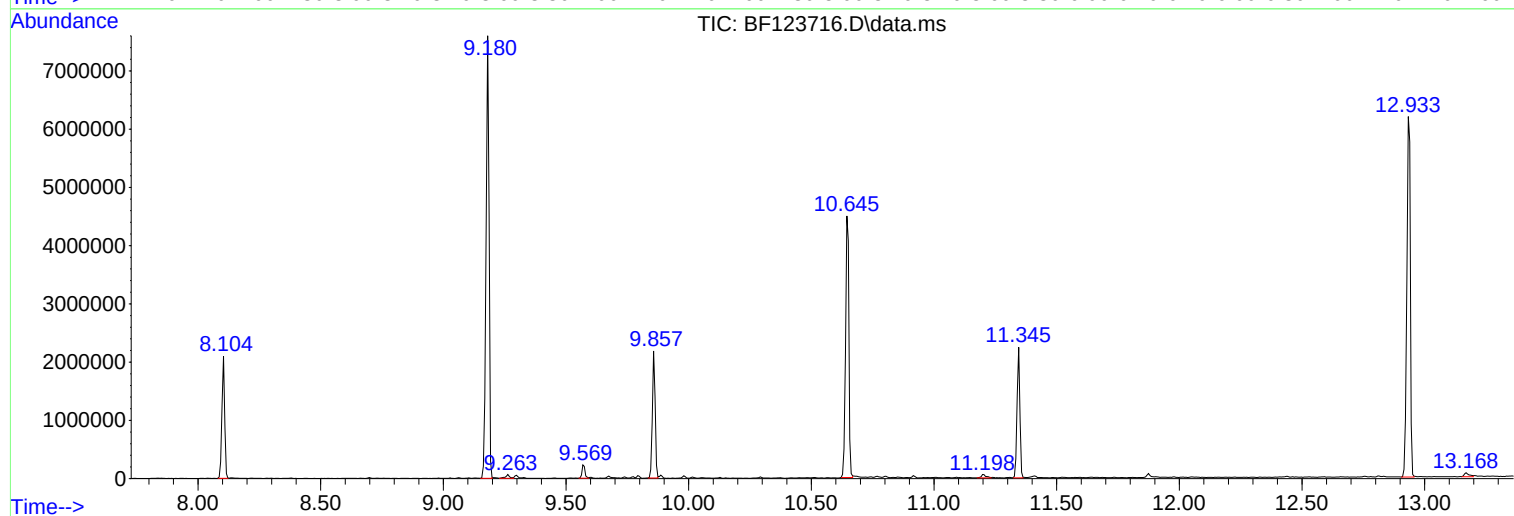
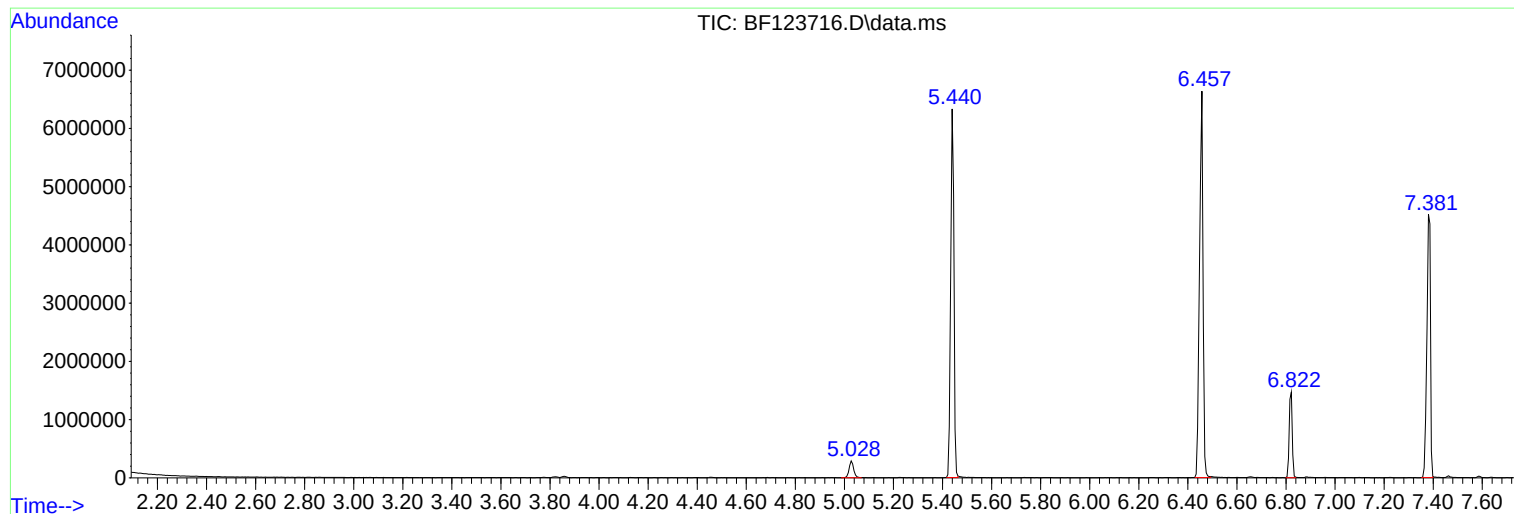
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SB-40-9.5-10.0

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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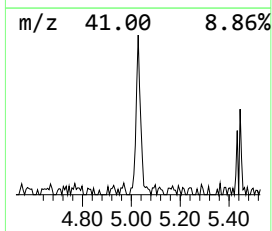
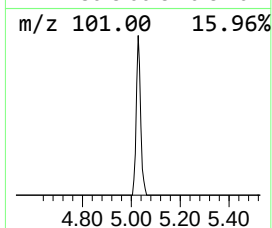
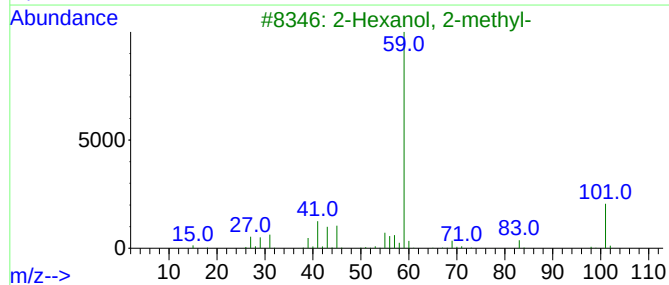
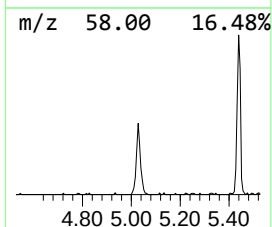
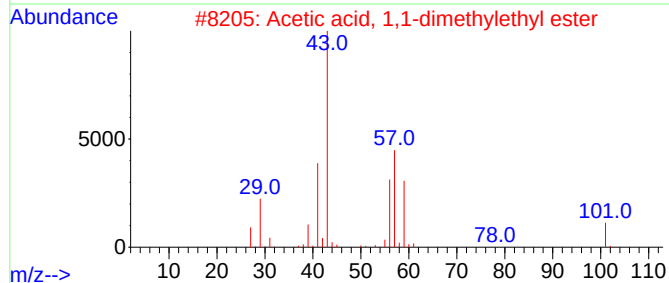
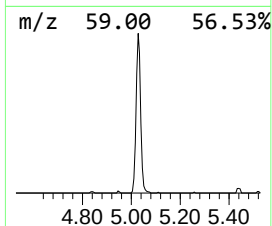
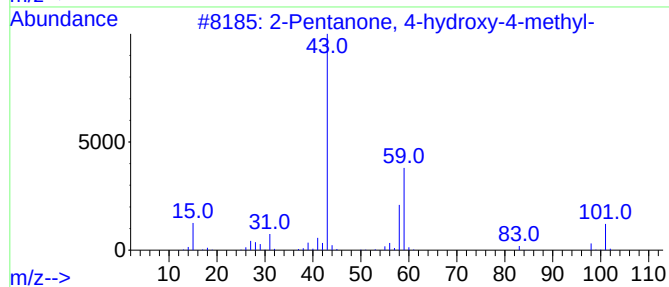
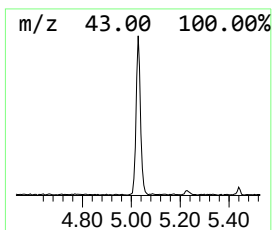
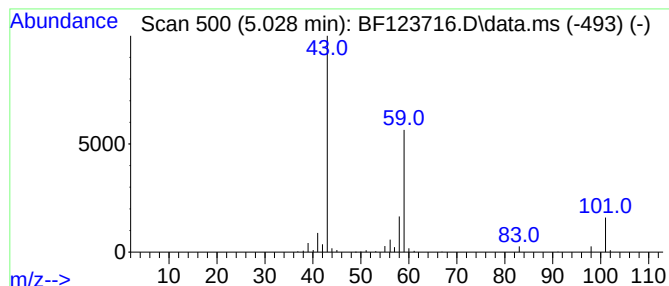
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.028	5.91 ng	375102	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	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Acetone	58	C3H6O	000067-64-1	9		



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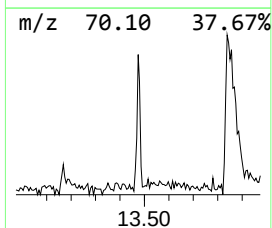
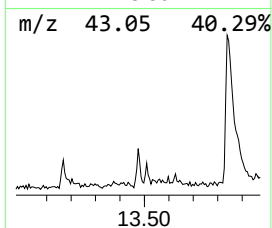
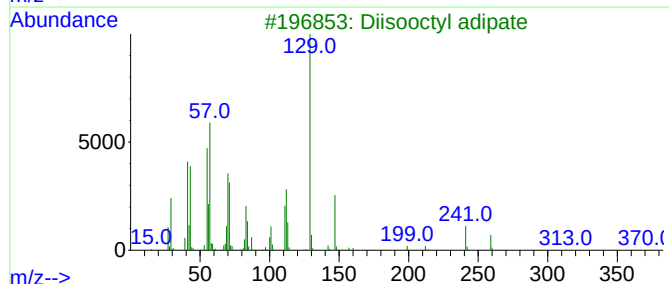
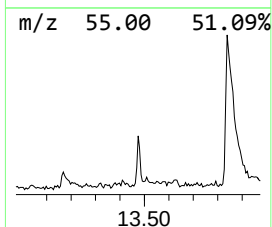
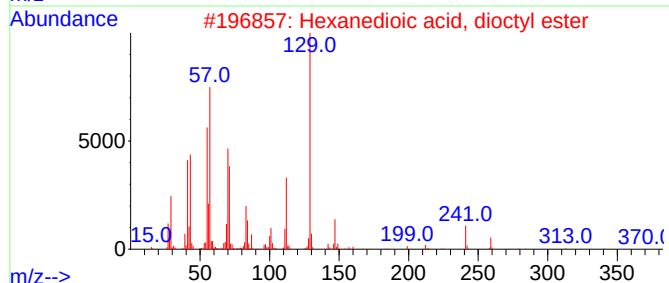
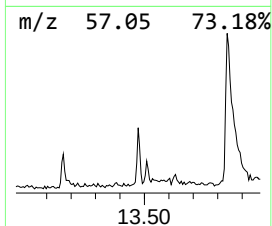
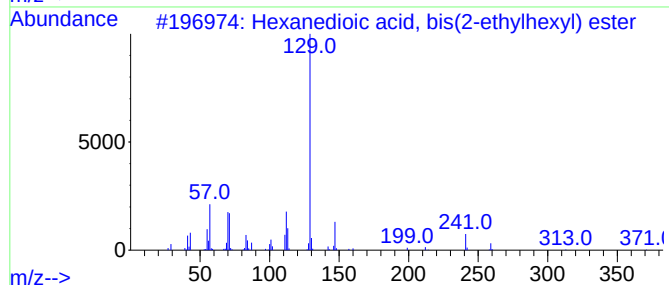
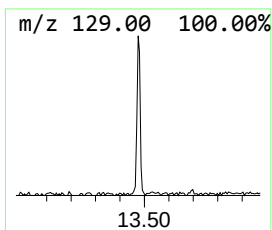
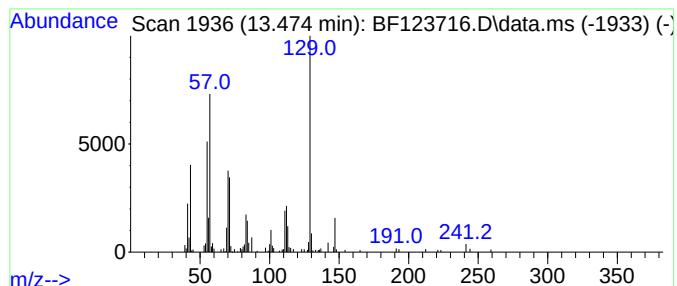
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	2.59 ng	185964	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	86
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58
3			Diisooctyl adipate	370	C22H42O4	001330-86-5	52
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	50
5			Adipic acid, octyl pent-4-en-2-y...	326	C19H34O4	1000354-12-4	43



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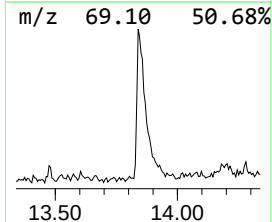
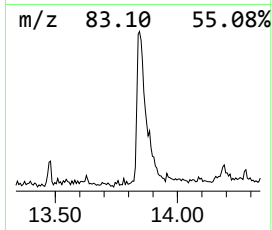
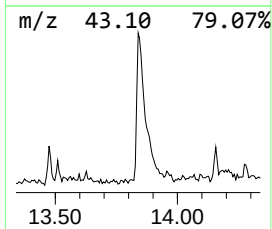
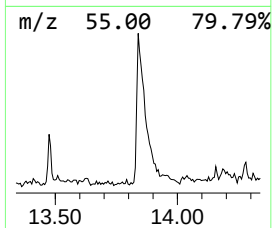
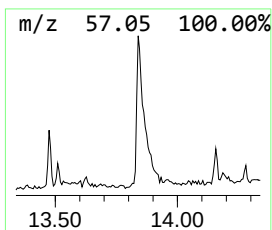
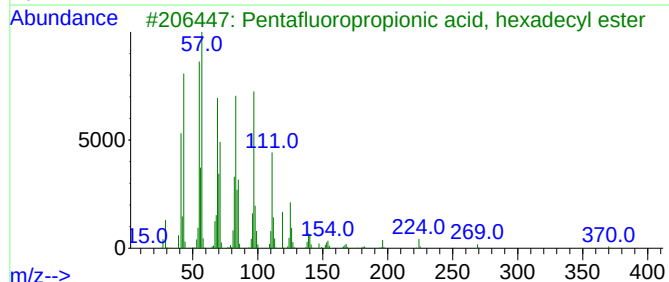
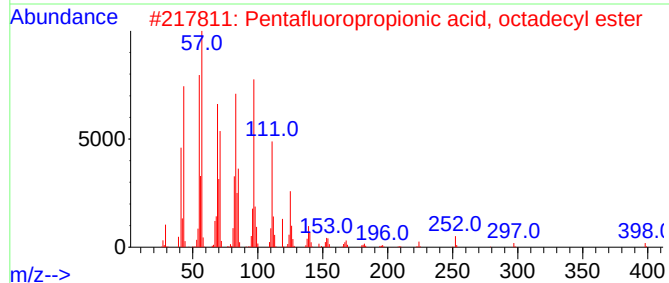
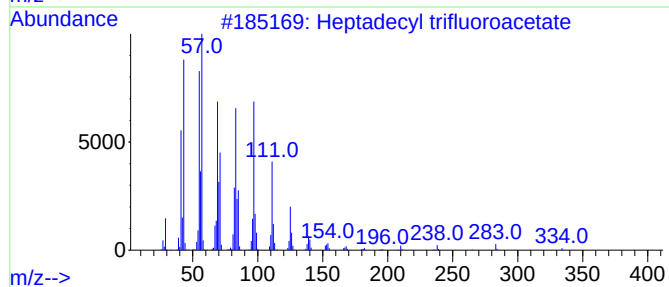
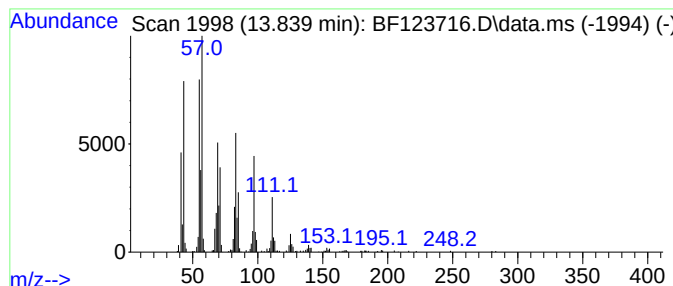
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	18.48 ng	1325940	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
3			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	91



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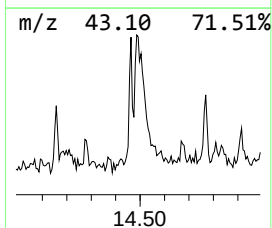
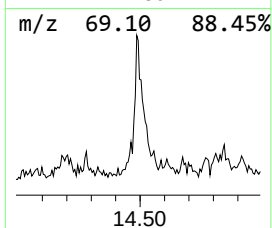
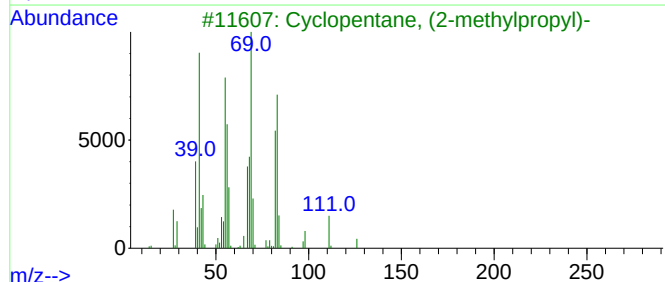
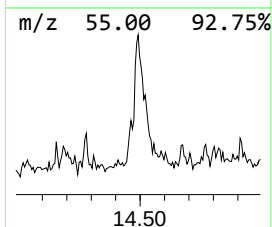
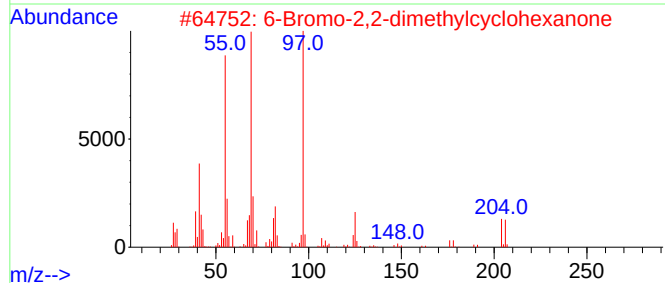
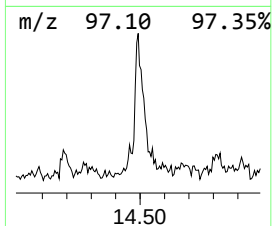
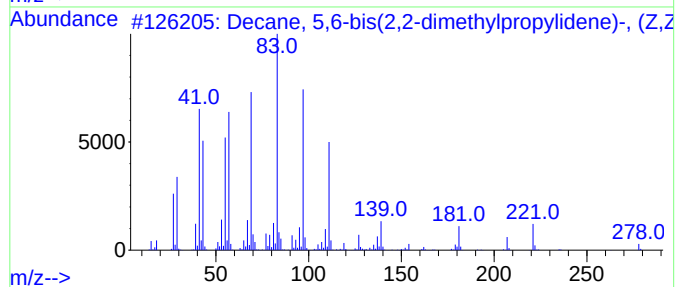
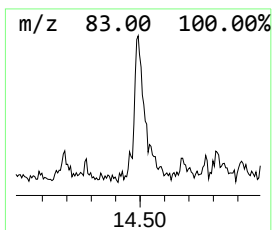
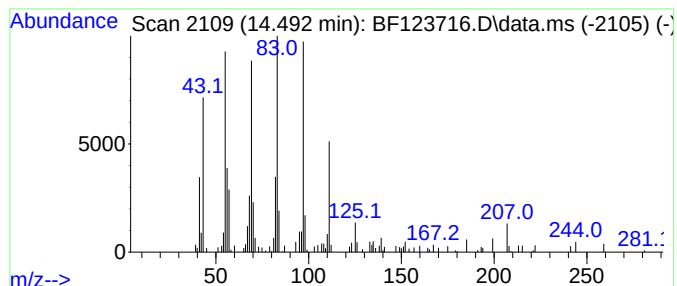
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Peak Number 4 Decane, 5,6-bis(2,2-dimethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.492	8.51 ng	610510	Chrysene-d12	13.986	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	59
2	6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	38
3	Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	38
4	3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	38
5	Hexahydropyrrolizin-3-one	125	C7H11NO	126424-83-7	38



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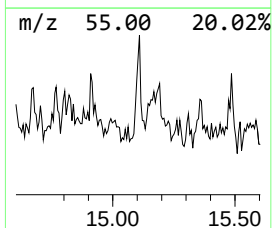
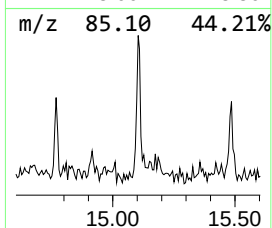
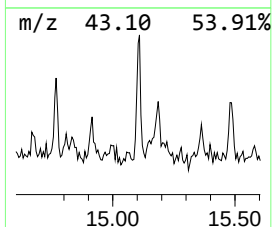
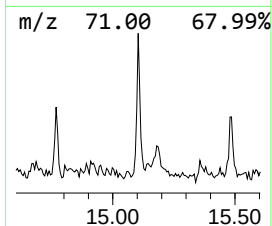
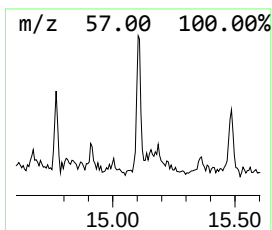
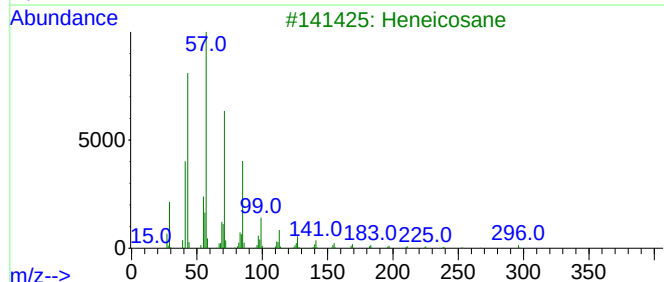
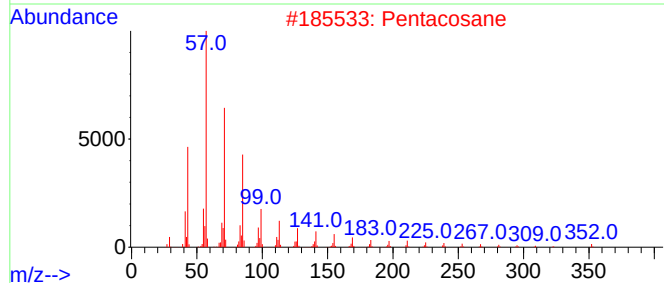
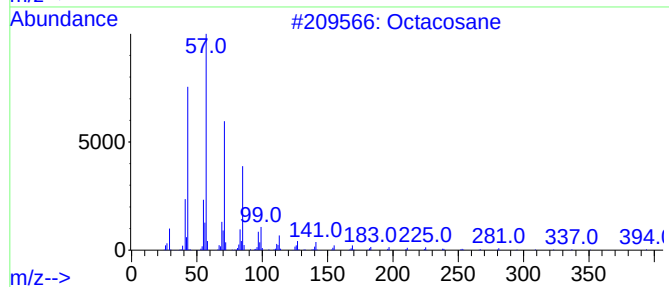
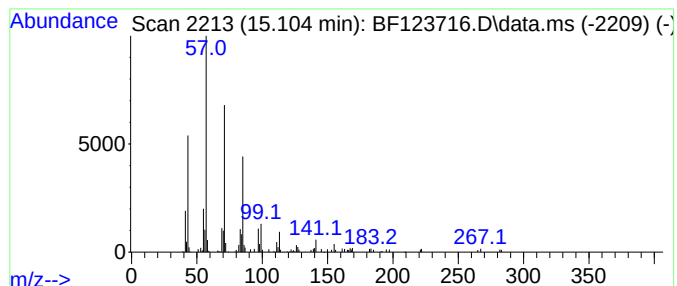
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	3.28 ng	179151	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Pentacosane	352	C25H52	000629-99-2	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Heptacosane	380	C27H56	000593-49-7	86
5			Tetracosane	338	C24H50	000646-31-1	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	5.9	ng	375102	1	6.822	1268360	20.0
Hexanedioic aci...	13.474	2.6	ng	185964	5	13.986	1435190	20.0
Heptadecyl trif...	13.839	18.5	ng	1325940	5	13.986	1435190	20.0
Decane, 5,6-bis...	14.492	8.5	ng	610510	5	13.986	1435190	20.0
Octacosane	15.104	3.3	ng	179151	6	15.445	1092940	20.0