

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123598.D
 Acq On : 16 Apr 2021 18:35
 Operator : JU/CG
 Sample : M2049-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-9.5-10.0

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: BF123598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	15	21	rVB	2734359	3595623	55.82%	6.965%
2	5.092	502	511	517	rBV	204196	260458	4.04%	0.505%
3	5.487	573	578	581	rBV	6376785	6085810	94.47%	11.788%
4	6.492	743	749	752	rBV	5778937	6310514	97.96%	12.224%
5	6.869	809	813	816	rBV	2077805	1664244	25.84%	3.224%
6	7.428	903	908	911	rBV	4435425	4190083	65.05%	8.116%
7	8.151	1026	1031	1034	rBV	2597521	2185426	33.93%	4.233%
8	9.233	1209	1215	1218	rBV	7515335	6441819	100.00%	12.478%
9	9.622	1278	1281	1285	rBV	281198	223555	3.47%	0.433%
10	9.910	1325	1330	1334	rBV	2541495	2347139	36.44%	4.546%
11	10.704	1460	1465	1468	rBV	4744335	4333974	67.28%	8.395%
12	11.404	1580	1584	1587	rBV	2639603	2404302	37.32%	4.657%
13	11.468	1590	1595	1597	rBV3	68399	73123	1.14%	0.142%
14	11.933	1670	1674	1684	rBV	380409	388888	6.04%	0.753%
15	12.721	1805	1808	1814	rBV	92536	100095	1.55%	0.194%
16	12.998	1850	1855	1858	rBV	6363854	5930915	92.07%	11.488%
17	13.909	2005	2010	2023	rBV4	282755	935998	14.53%	1.813%
18	14.051	2029	2034	2037	rBV	1955053	1774617	27.55%	3.437%
19	14.221	2059	2063	2066	rBV	121945	104851	1.63%	0.203%
20	14.527	2111	2115	2118	rBV	141353	127869	1.98%	0.248%
21	14.839	2165	2168	2173	rVB2	135212	128754	2.00%	0.249%
22	15.186	2223	2227	2233	rBV	167919	187727	2.91%	0.364%
23	15.533	2281	2286	2291	rBV	1013379	1349838	20.95%	2.615%
24	15.580	2291	2294	2302	rVB	121797	173928	2.70%	0.337%
25	16.027	2365	2370	2376	rBV	94774	150462	2.34%	0.291%
26	16.151	2382	2391	2396	rBV	24046	74020	1.15%	0.143%
27	16.545	2453	2458	2463	rBV3	44521	81220	1.26%	0.157%

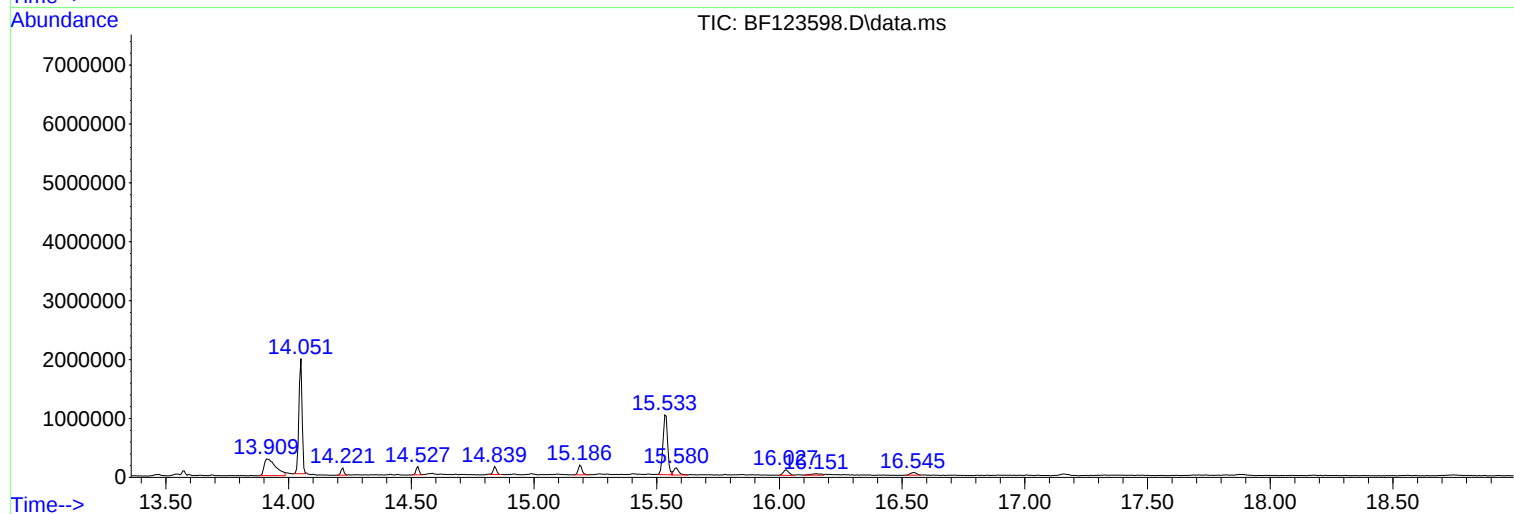
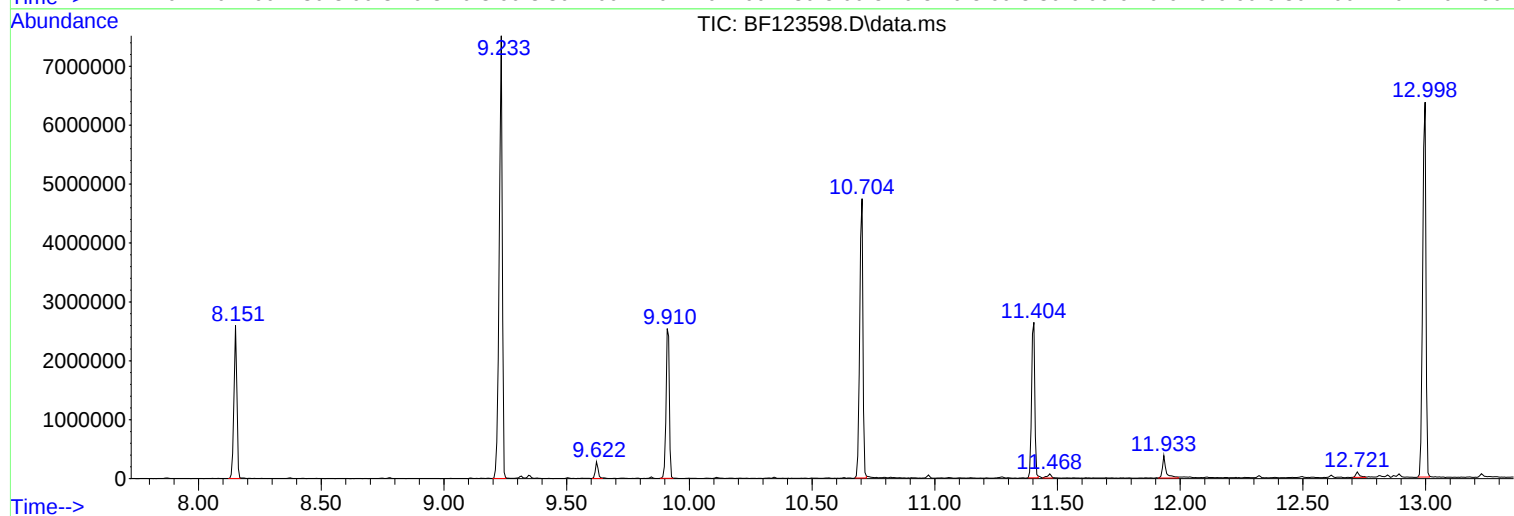
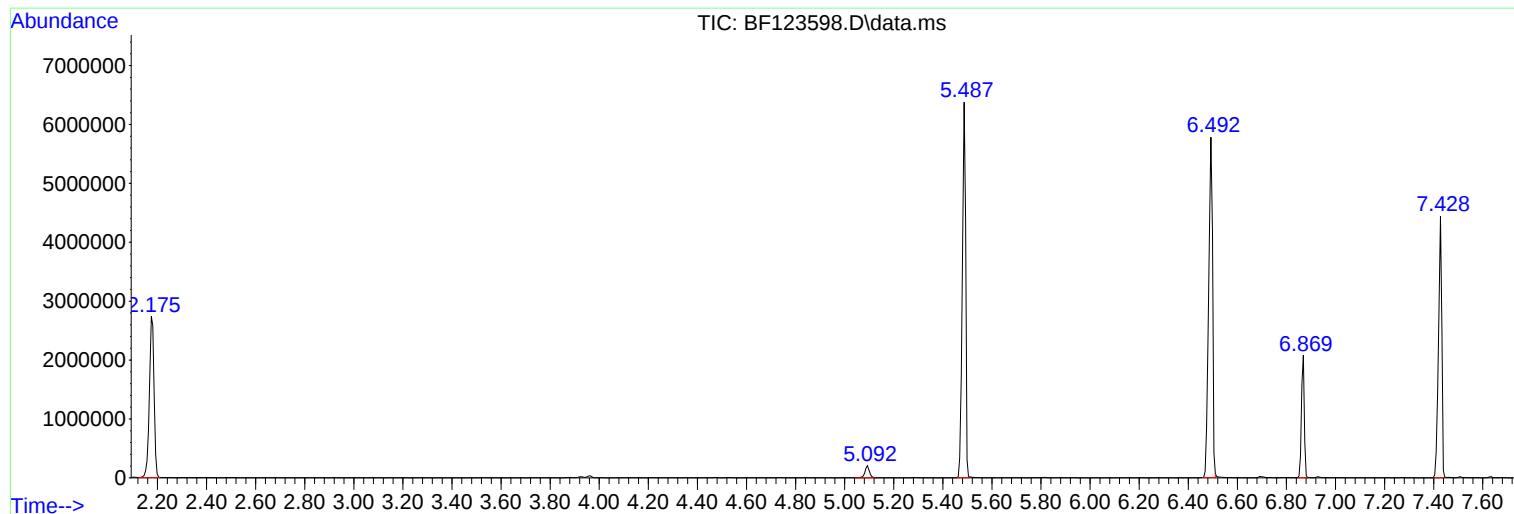
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ClientSampleId :
SB-07-9.5-10.0

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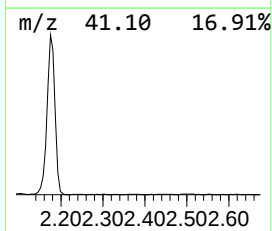
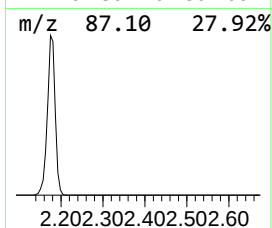
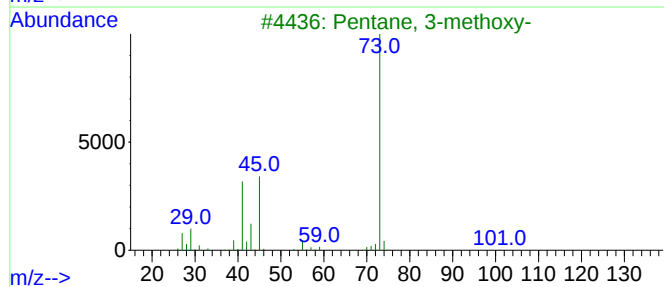
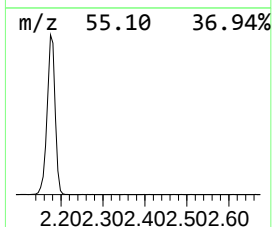
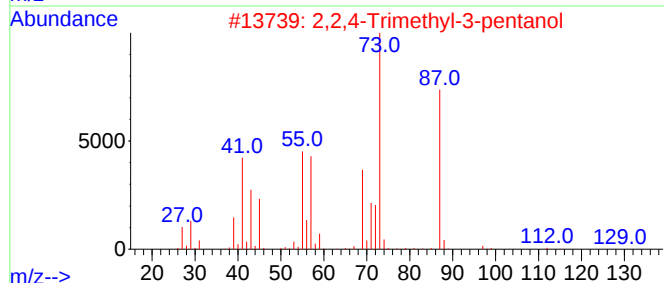
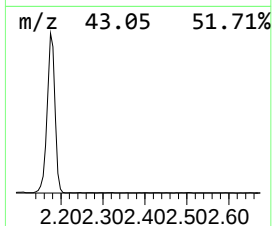
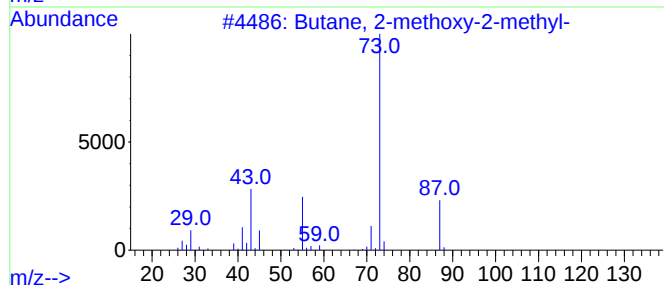
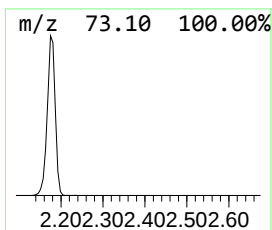
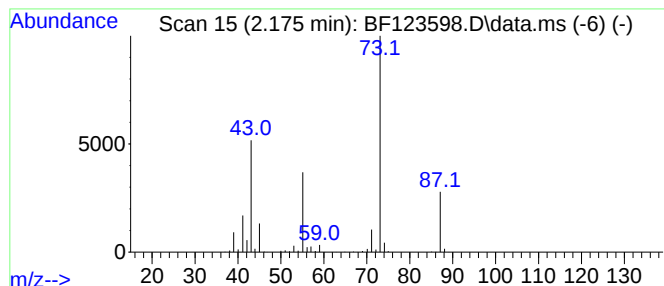
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	43.21 ng	3595620	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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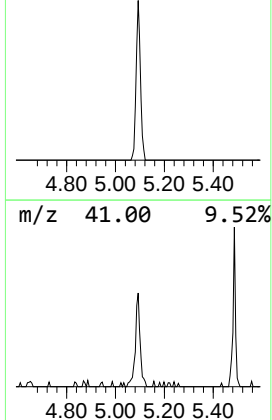
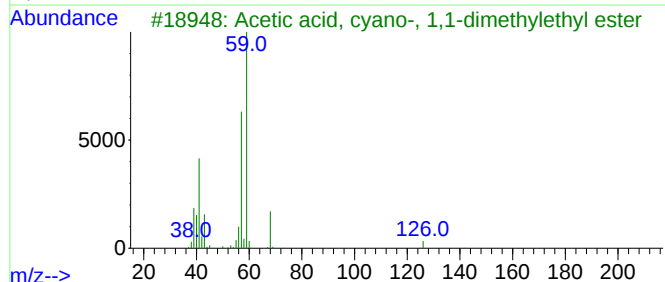
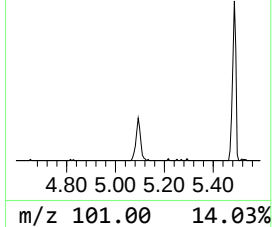
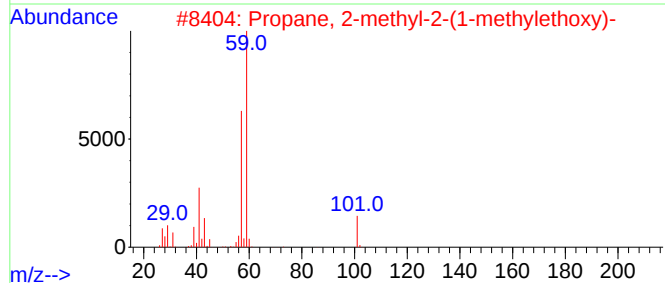
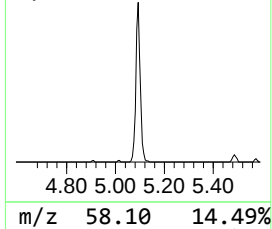
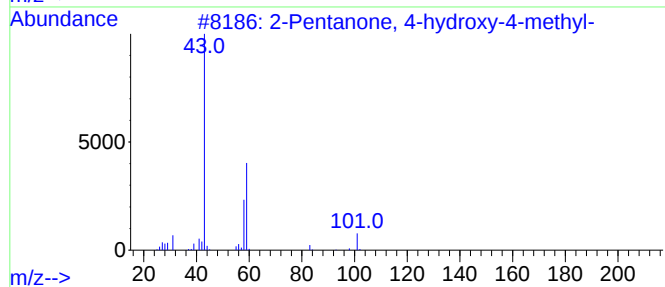
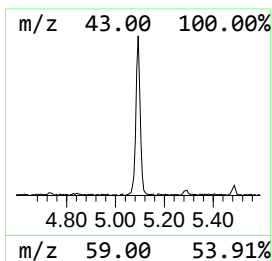
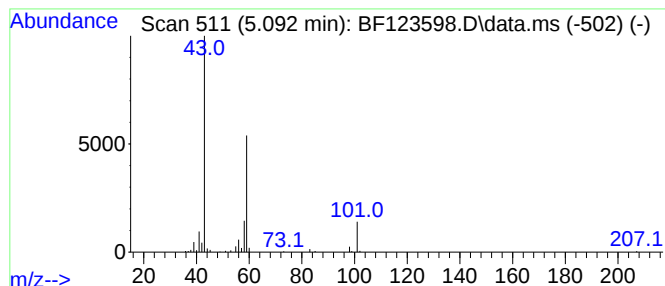
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	3.13 ng	260458	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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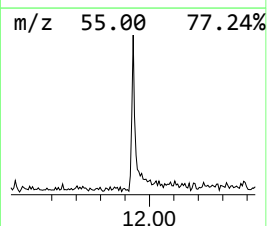
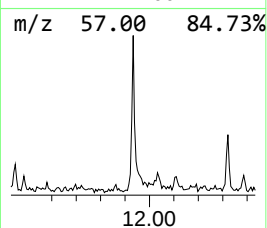
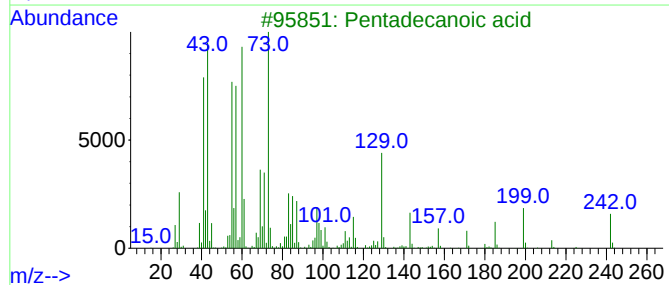
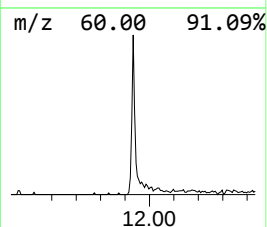
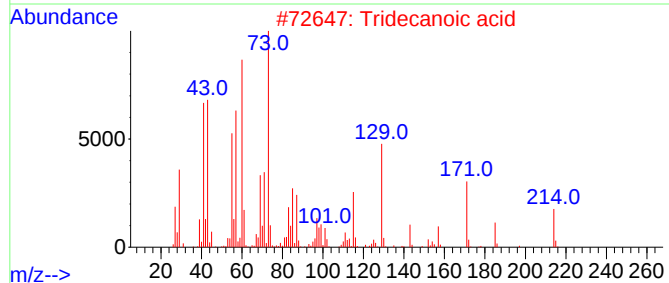
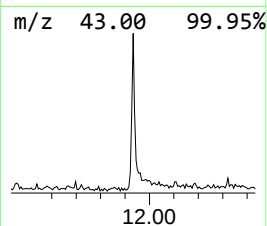
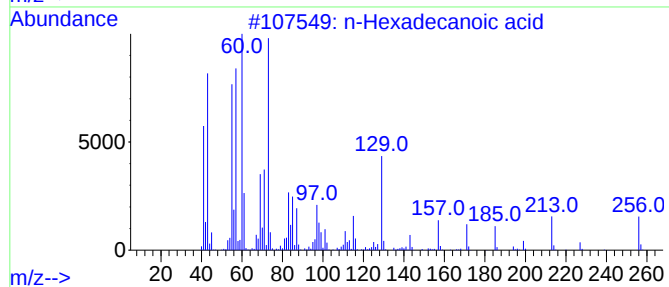
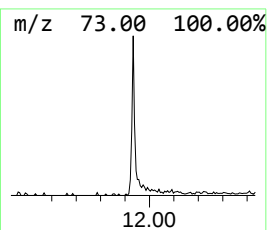
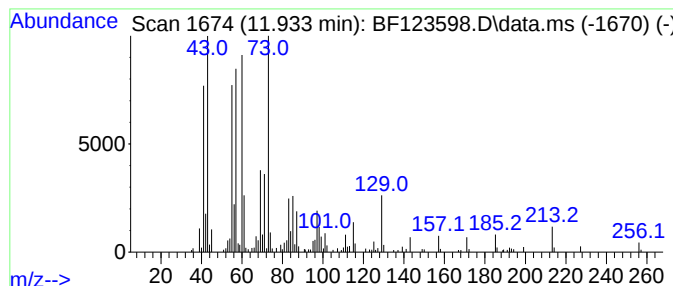
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.23 ng	388888	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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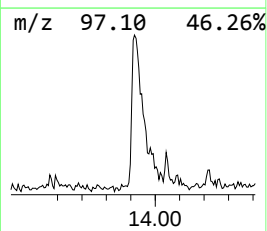
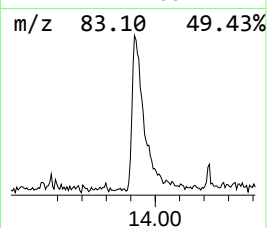
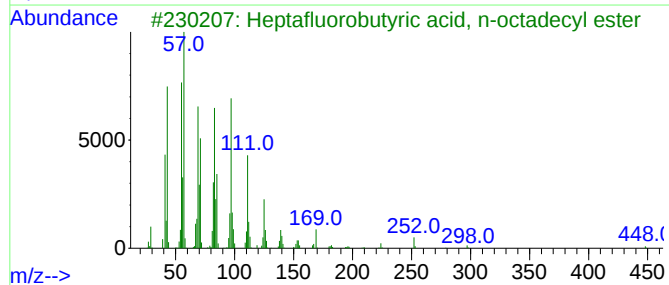
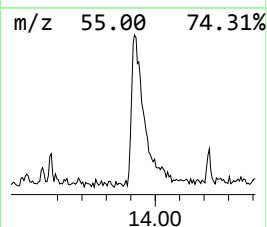
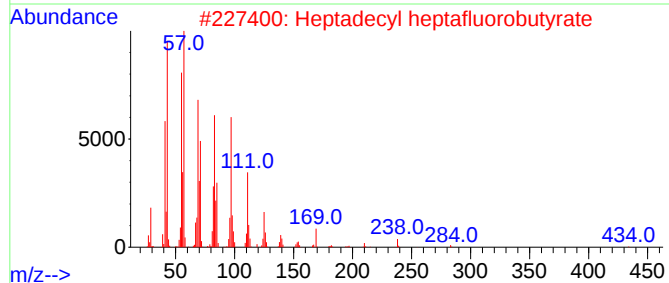
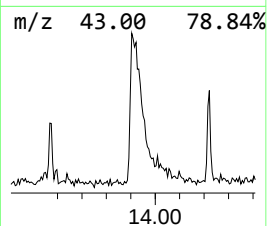
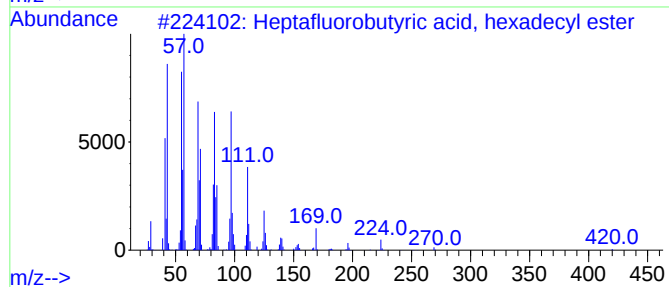
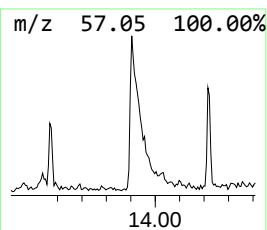
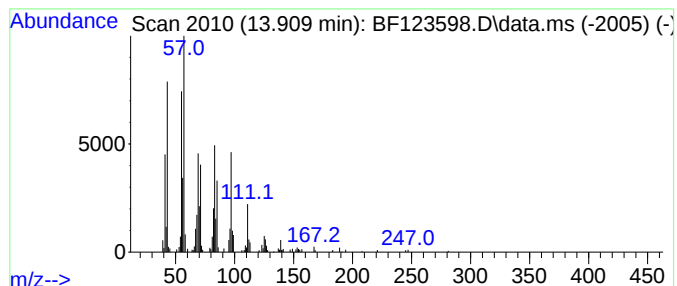
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Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	10.55 ng	935998	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



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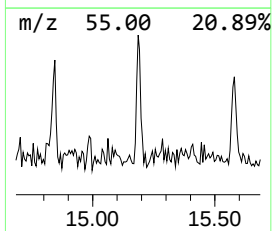
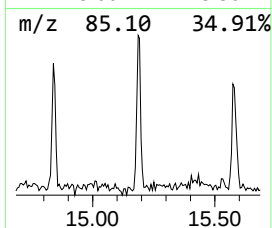
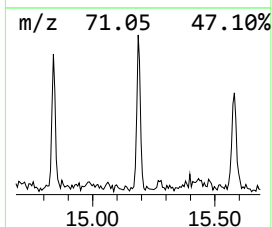
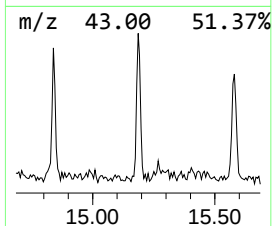
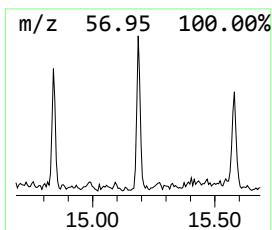
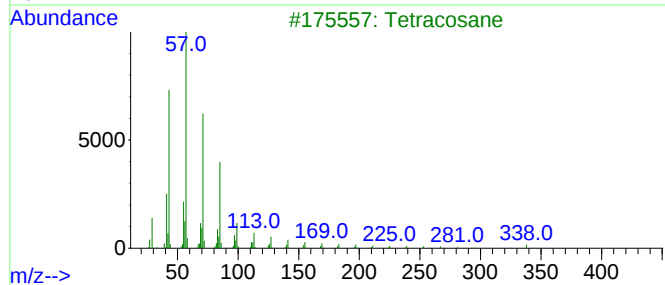
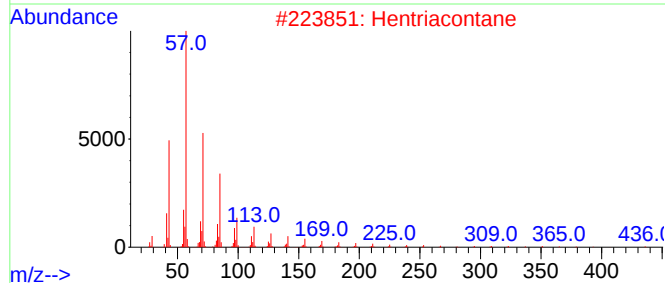
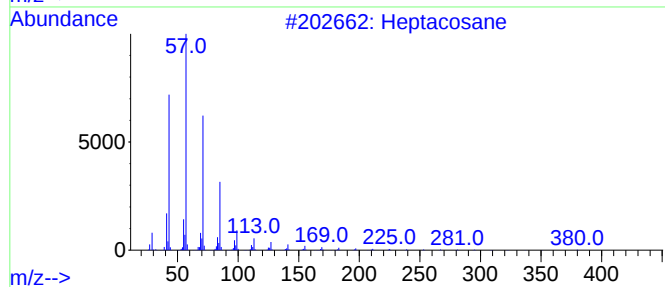
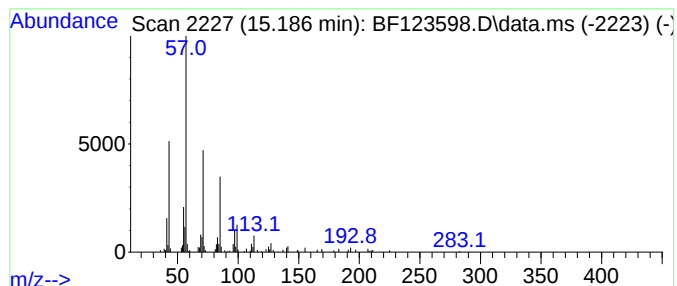
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	2.78 ng	187727	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Hexacosane	366	C26H54	000630-01-3	83
5	Octacosane	394	C28H58	000630-02-4	81



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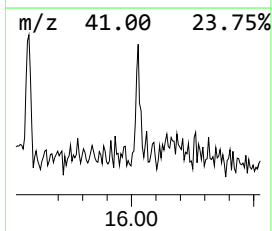
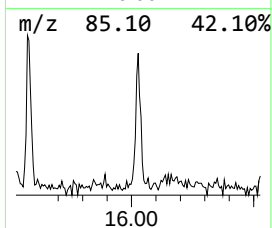
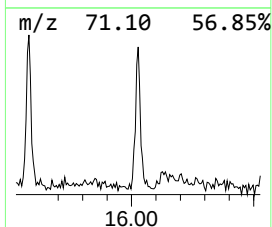
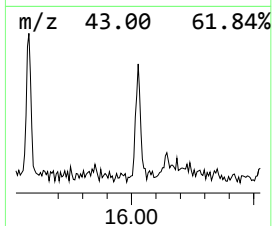
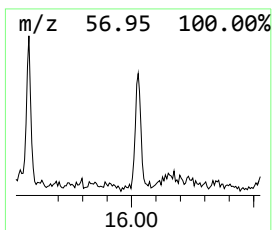
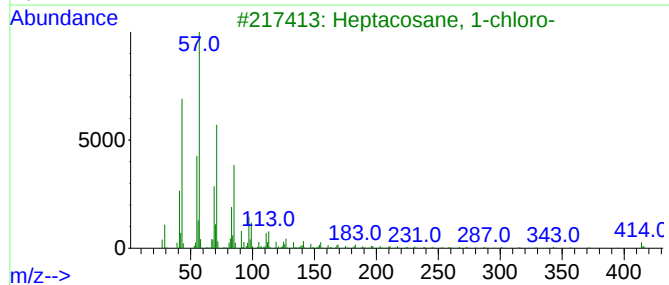
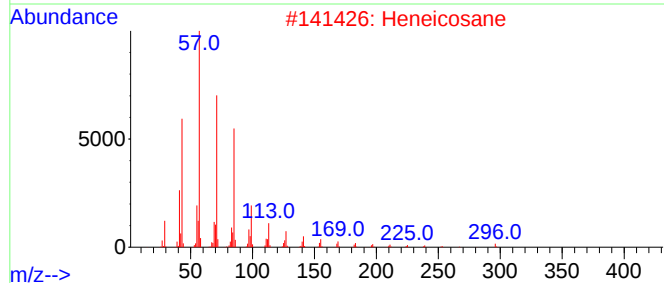
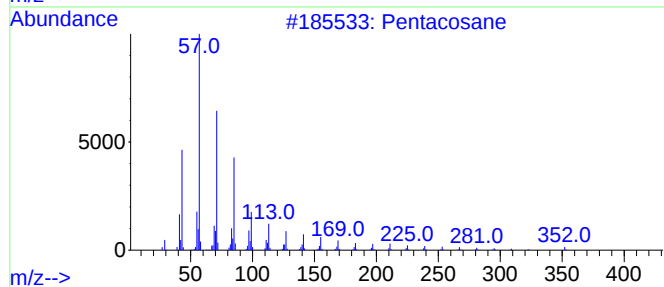
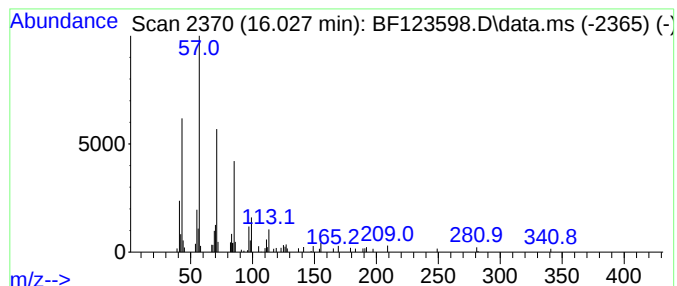
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	2.23 ng	150462	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	86
2			Heneicosane	296	C21H44	000629-94-7	86
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123598.D
Acq On : 16 Apr 2021 18:35
Operator : JU/CG
Sample : M2049-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-9.5-10.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	43.2	ng	3595620	1	6.869	1664240	20.0
2-Pentanone, 4-...	5.092	3.1	ng	260458	1	6.869	1664240	20.0
n-Hexadecanoic ...	11.933	3.2	ng	388888	4	11.404	2404300	20.0
Heptafluorobuty...	13.910	10.6	ng	935998	5	14.051	1774620	20.0
Heptacosane	15.186	2.8	ng	187727	6	15.533	1349840	20.0
Pentacosane	16.027	2.2	ng	150462	6	15.533	1349840	20.0