

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
 Data File : BF122952.D
 Acq On : 8 Jan 2021 21:06
 Operator : JU/CG
 Sample : M1044-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10

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-BF010721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	18	23	32	rVB	527836	732076	15.98%	2.103%
2	2.334	38	42	50	rVB2	65371	93168	2.03%	0.268%
3	3.428	224	228	238	rBV	22835	47573	1.04%	0.137%
4	5.140	510	519	525	rVB	331701	395808	8.64%	1.137%
5	5.534	581	586	589	rBV	4213948	4121302	89.97%	11.841%
6	6.534	750	756	766	rBV	3941325	4211149	91.93%	12.099%
7	6.916	817	821	824	rBV	1495508	1131245	24.70%	3.250%
8	7.475	911	916	919	rBV	2810435	2560358	55.89%	7.356%
9	8.198	1035	1039	1043	rBV	1753473	1452068	31.70%	4.172%
10	9.281	1218	1223	1226	rBV	4912146	4580735	100.00%	13.161%
11	9.363	1232	1237	1245	rBV4	72396	105161	2.30%	0.302%
12	9.669	1285	1289	1293	rBV	213856	192853	4.21%	0.554%
13	9.757	1298	1304	1311	rVB4	40088	49720	1.09%	0.143%
14	9.957	1334	1338	1342	rBV	1828466	1542544	33.67%	4.432%
15	10.745	1467	1472	1475	rBV	3009319	2598132	56.72%	7.465%
16	11.310	1562	1568	1572	rBV4	45401	66768	1.46%	0.192%
17	11.445	1588	1591	1594	rBV	1536018	1422576	31.06%	4.087%
18	11.975	1675	1681	1685	rBV2	182104	207628	4.53%	0.597%
19	12.069	1694	1697	1705	rVB5	28324	51470	1.12%	0.148%
20	12.280	1729	1733	1736	rVB	42357	50196	1.10%	0.144%
21	12.439	1756	1760	1763	rBV	244241	226562	4.95%	0.651%
22	12.492	1766	1769	1773	rBV2	75516	75730	1.65%	0.218%
23	12.663	1795	1798	1801	rBV	164692	136627	2.98%	0.393%
24	12.892	1833	1837	1840	rBV	131228	121698	2.66%	0.350%
25	13.039	1858	1862	1866	rBV	4454829	4138123	90.34%	11.890%
26	13.939	2011	2015	2023	rBV	586224	550402	12.02%	1.581%
27	14.098	2037	2042	2045	rBV	1681095	1544270	33.71%	4.437%
28	14.263	2068	2070	2076	rVB2	36892	48921	1.07%	0.141%
29	14.574	2121	2123	2127	rVB2	79903	75307	1.64%	0.216%
30	14.968	2187	2190	2196	rVB	191808	189073	4.13%	0.543%
31	15.145	2217	2220	2224	rBV	67572	110363	2.41%	0.317%
32	15.457	2271	2273	2280	rVB	58462	68771	1.50%	0.198%
33	15.521	2281	2284	2287	rVB	54550	63474	1.39%	0.182%
34	15.592	2290	2296	2300	rBV	1264234	1562834	34.12%	4.490%
35	16.086	2378	2380	2384	rVB	48603	60242	1.32%	0.173%
36	16.139	2385	2389	2400	rVB6	86987	169400	3.70%	0.487%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.615	2468	2470	2474	rVB2	39626	50222	1.10%	0.144%
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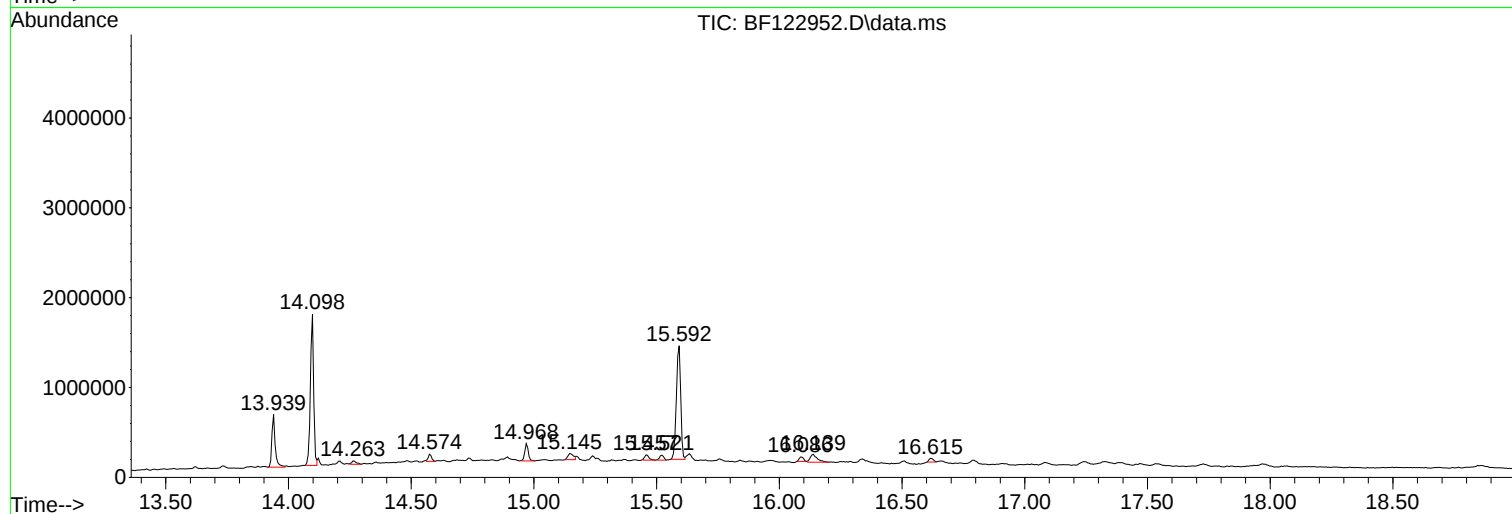
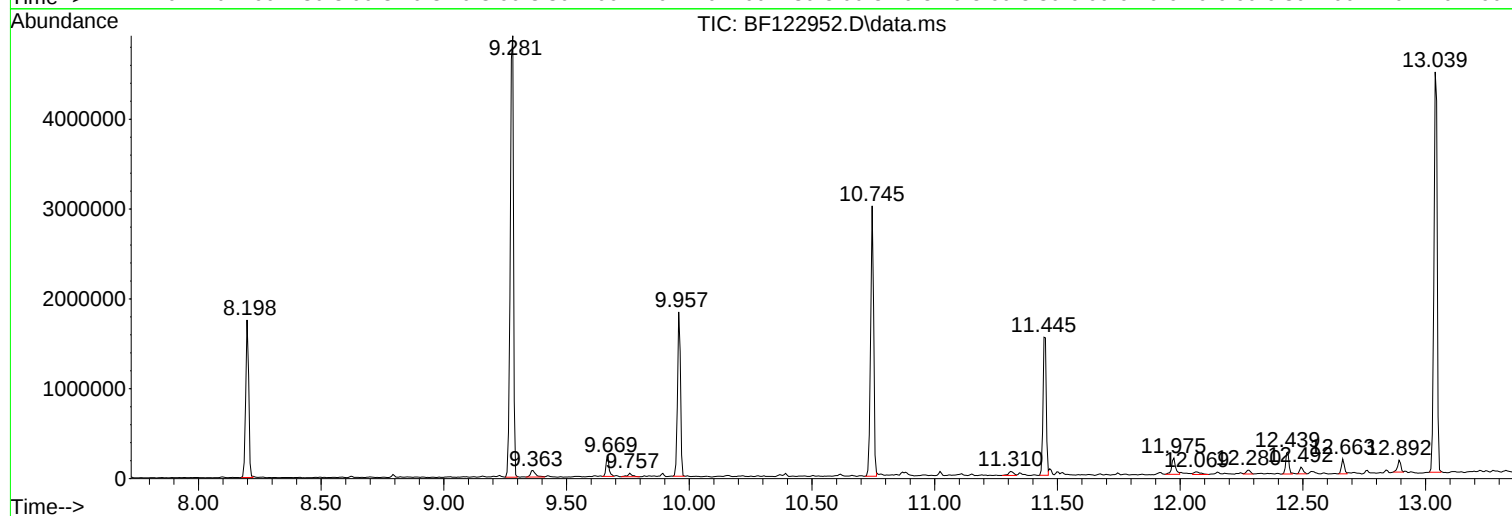
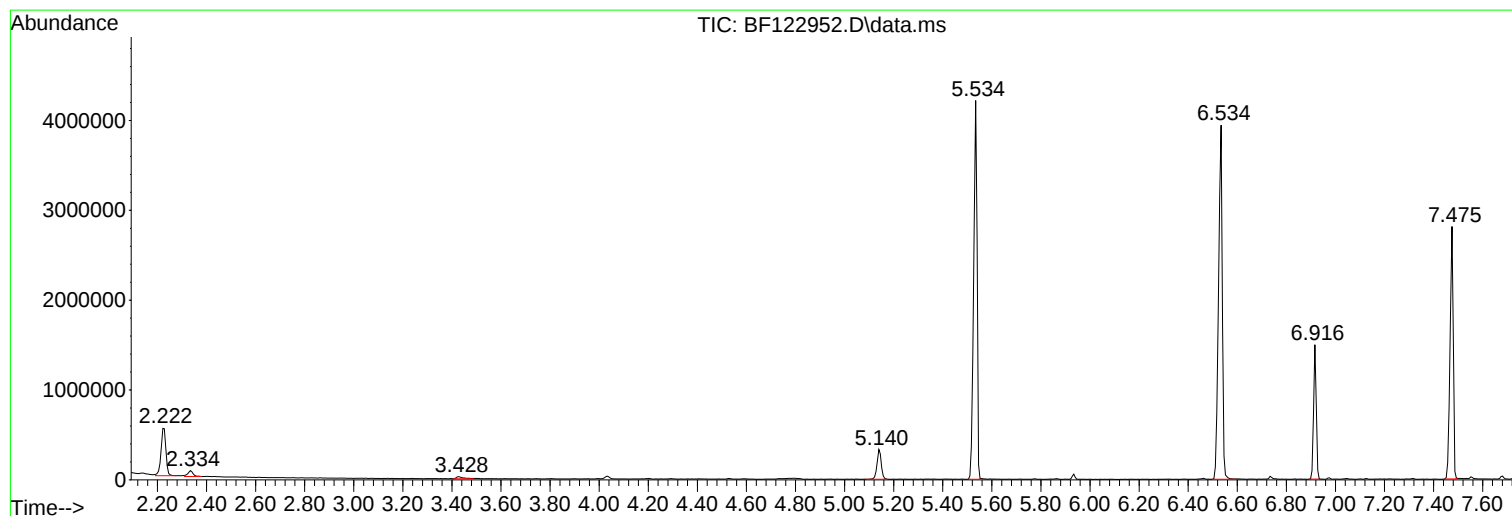
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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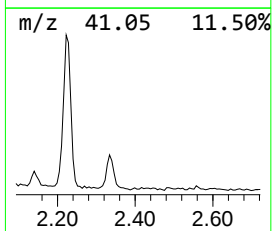
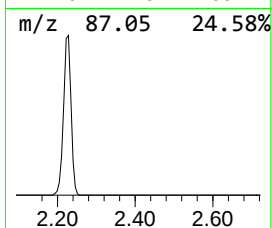
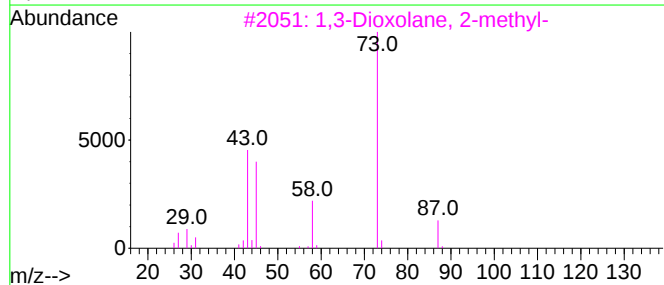
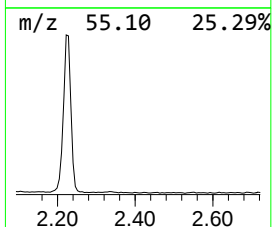
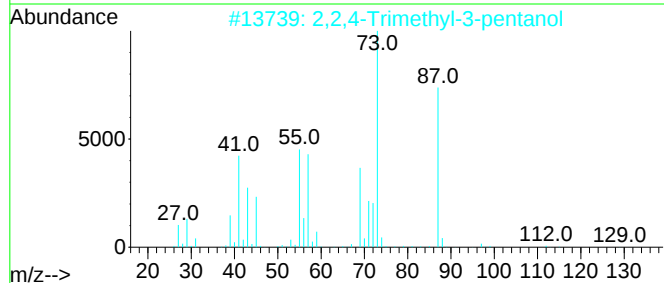
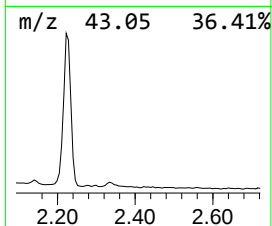
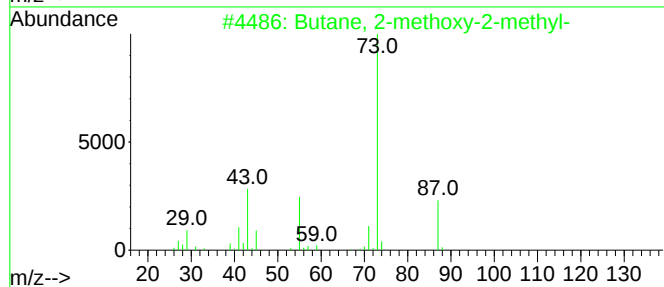
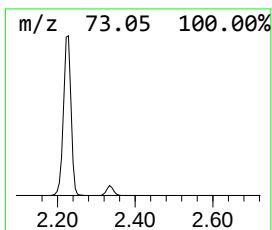
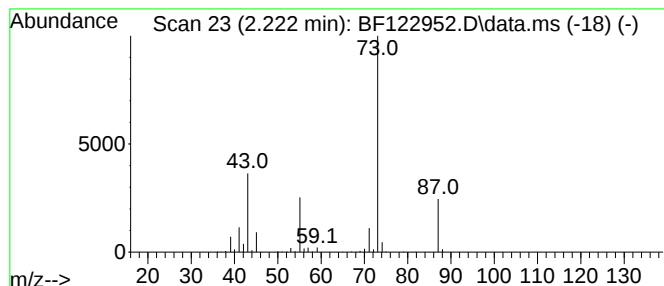
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	12.94 ng	732076	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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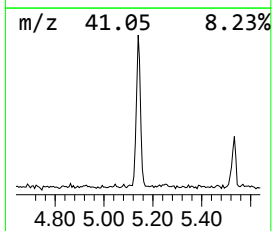
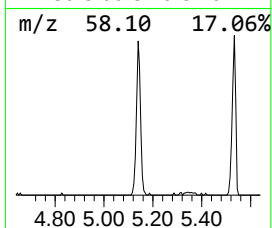
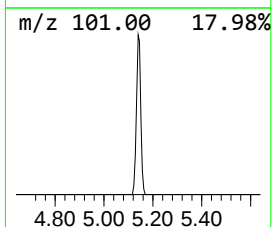
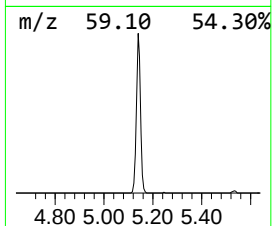
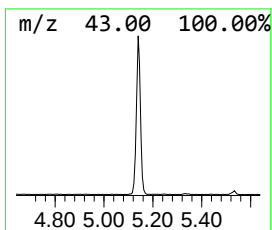
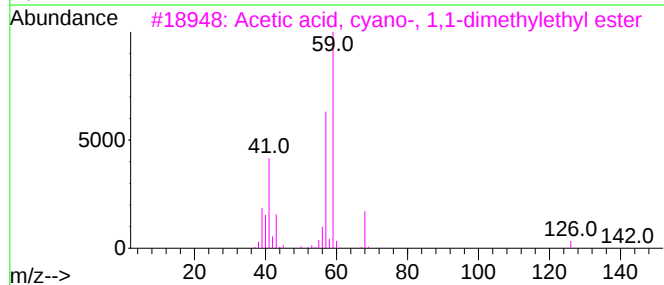
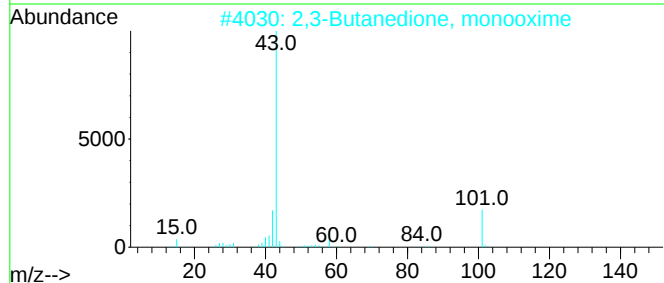
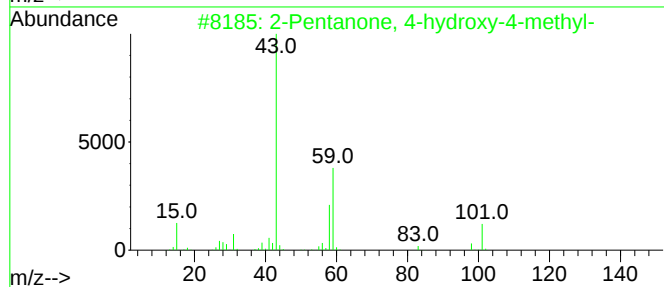
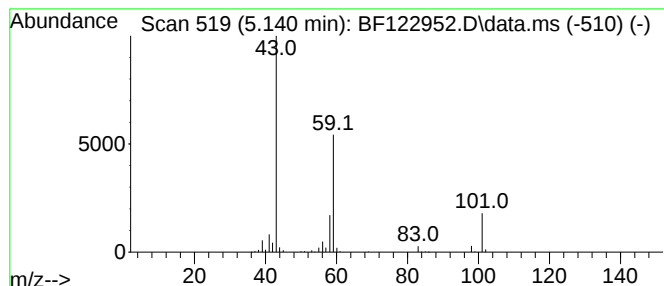
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	7.00 ng	395808	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Acetone	58	C3H6O	000067-64-1	9



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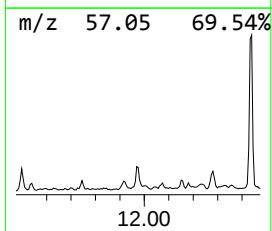
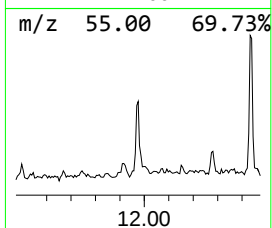
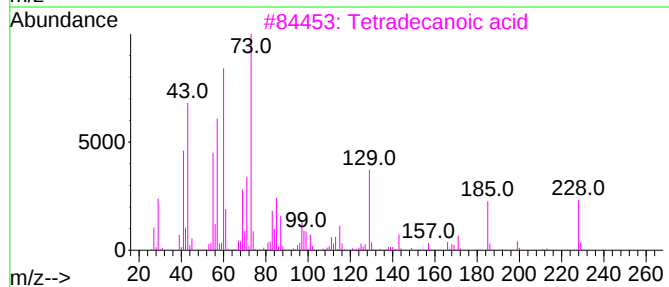
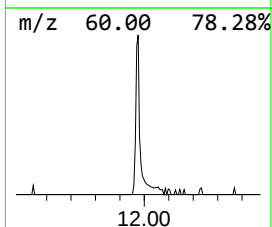
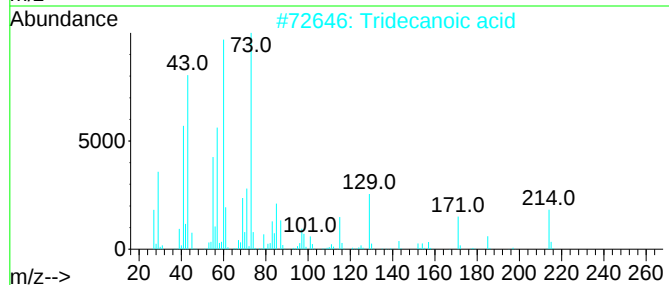
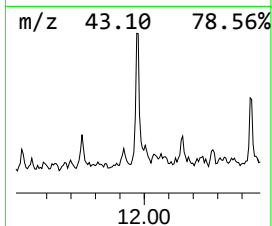
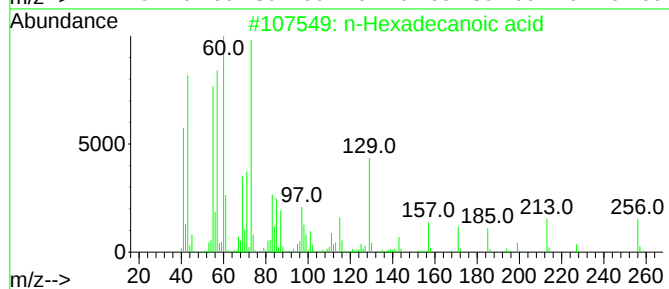
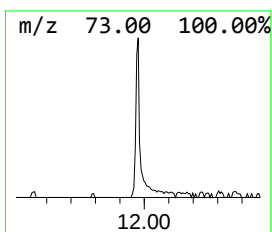
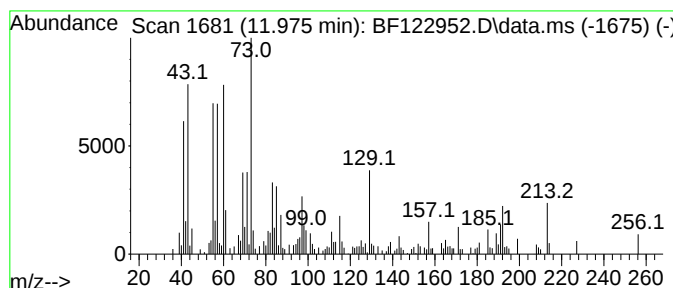
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.975	2.92 ng	207628	Phenanthrene-d10	11.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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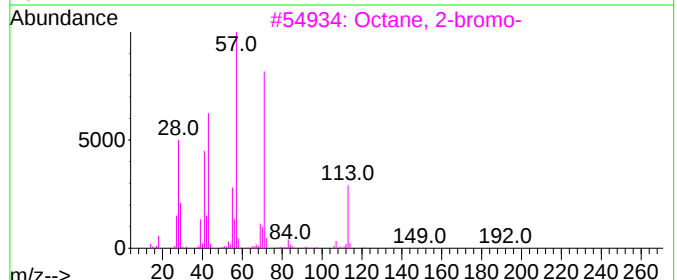
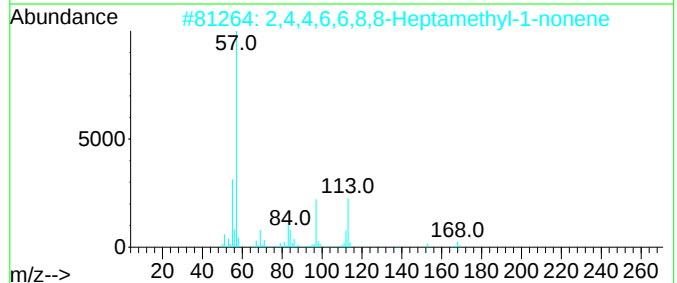
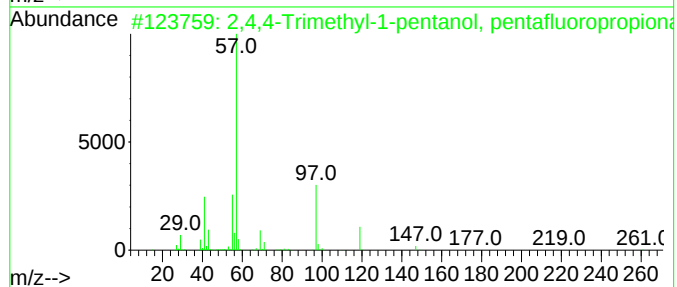
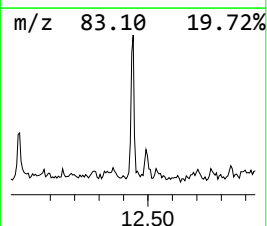
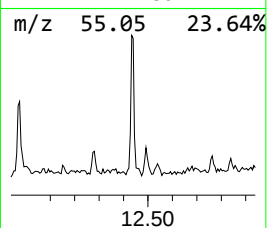
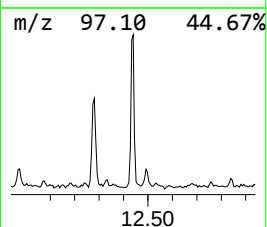
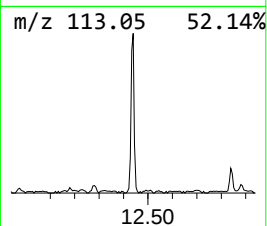
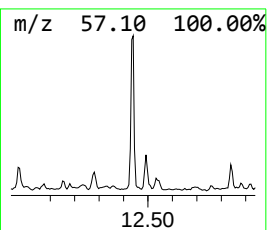
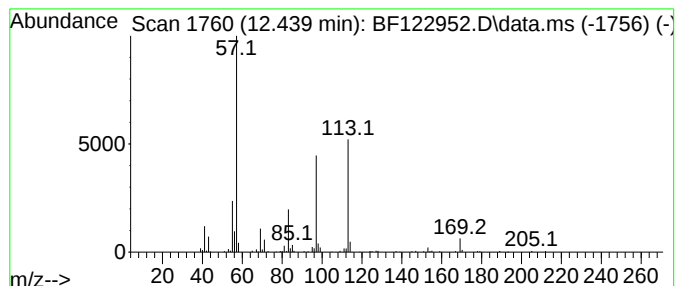
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.439 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.439	3.19 ng	226562	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38
2			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
3			Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
4			2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
5			2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25



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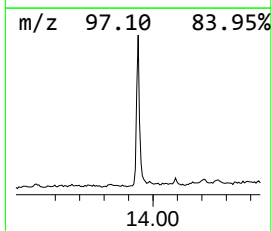
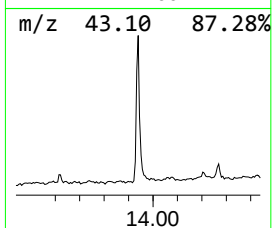
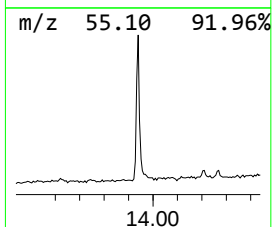
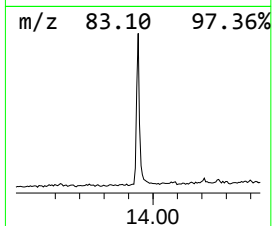
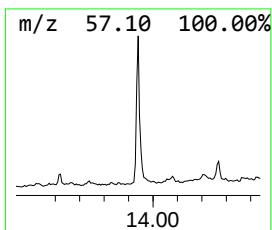
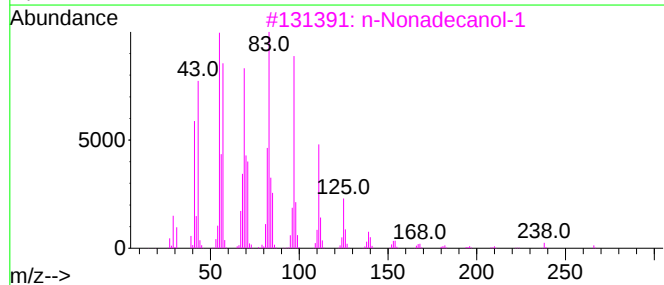
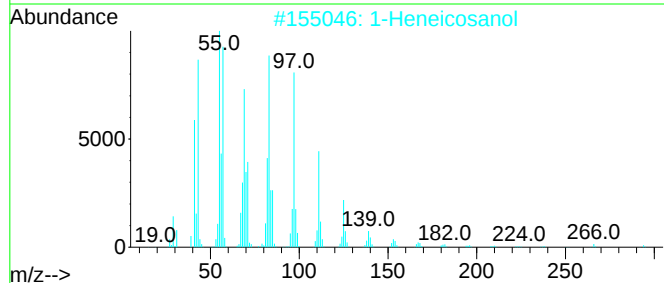
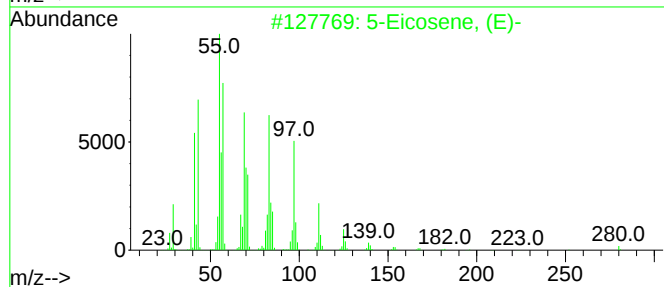
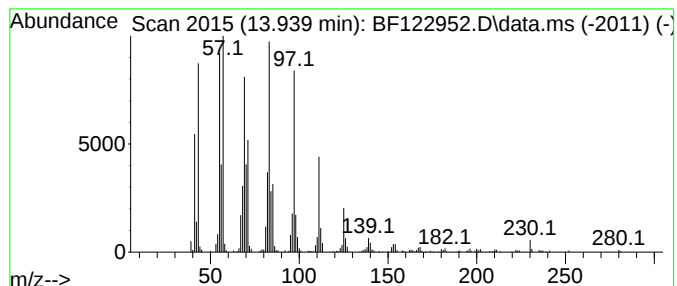
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	7.13 ng	550402	Chrysene-d12	14.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Cyclopentadecane	210	C15H30	000295-48-7	94
5		Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122952.D
Acq On : 8 Jan 2021 21:06
Operator : JU/CG
Sample : M1044-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

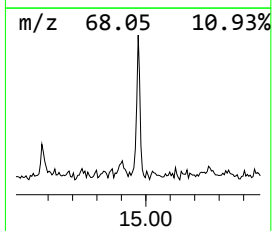
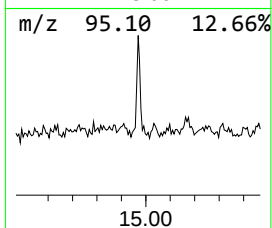
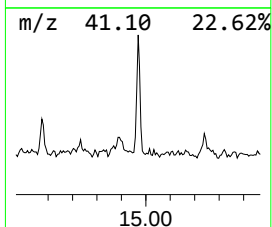
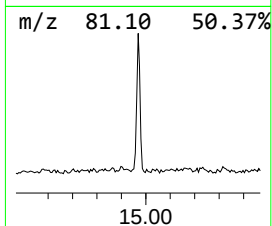
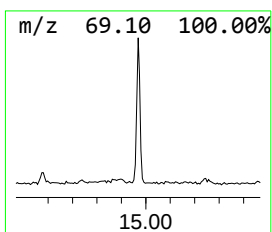
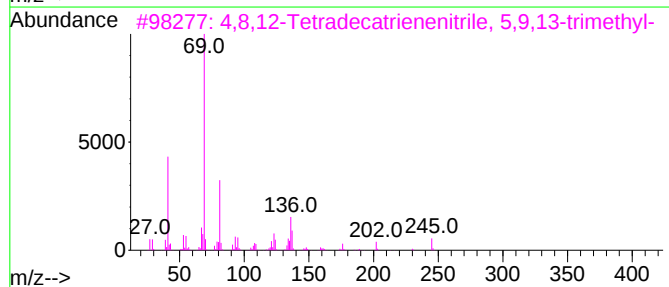
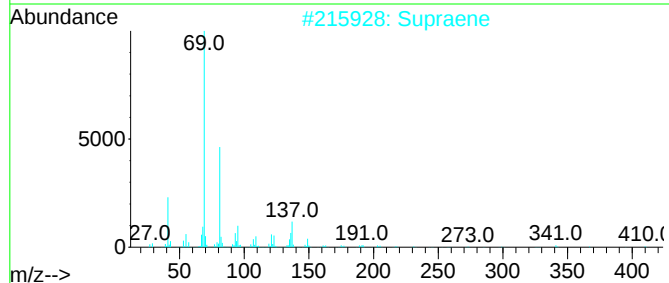
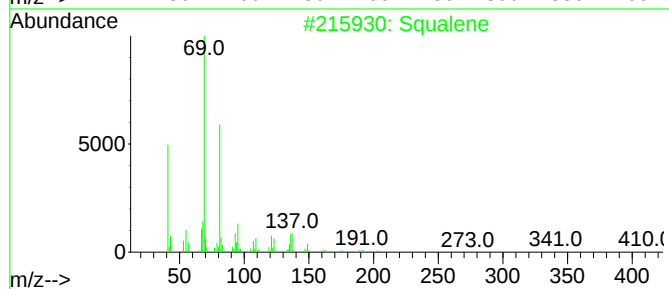
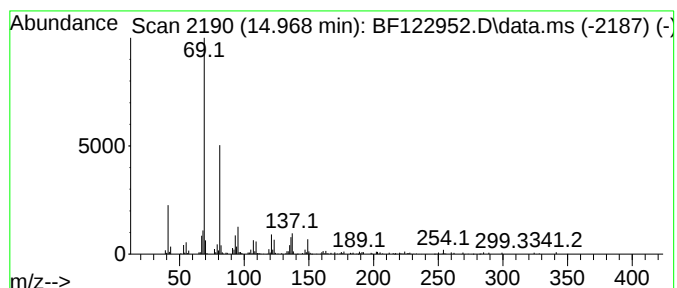
Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.969	2.42 ng	189073	Perylene-d12	15.592	
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	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122952.D
Acq On : 8 Jan 2021 21:06
Operator : JU/CG
Sample : M1044-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

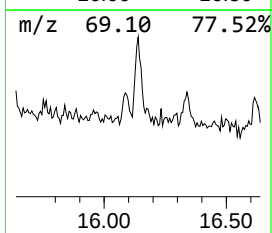
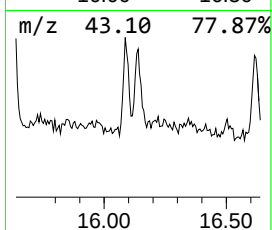
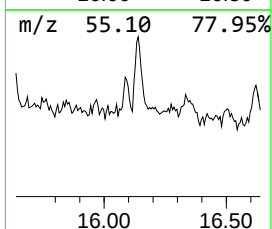
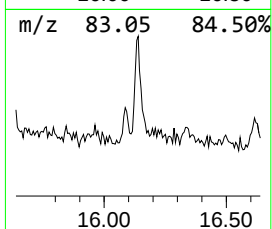
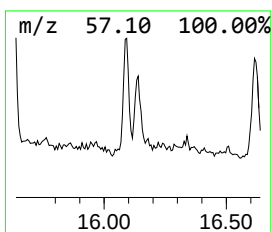
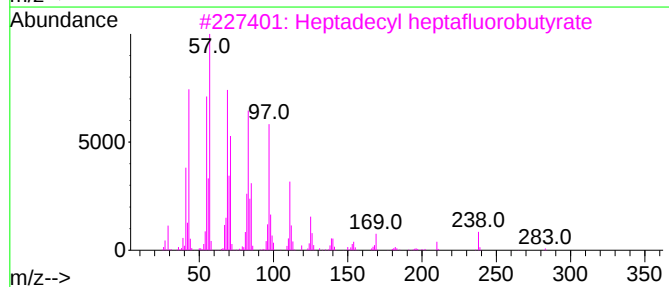
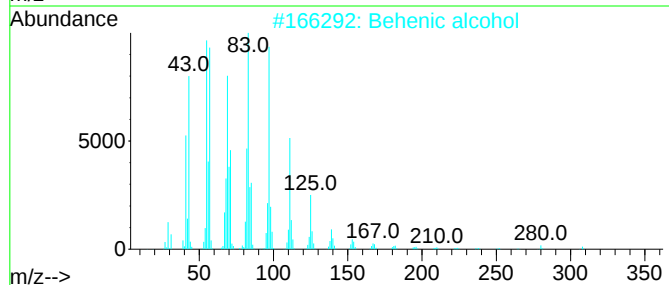
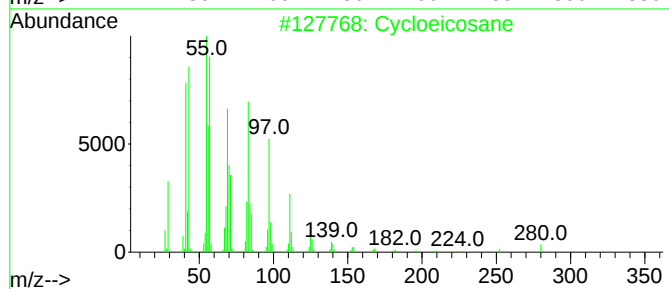
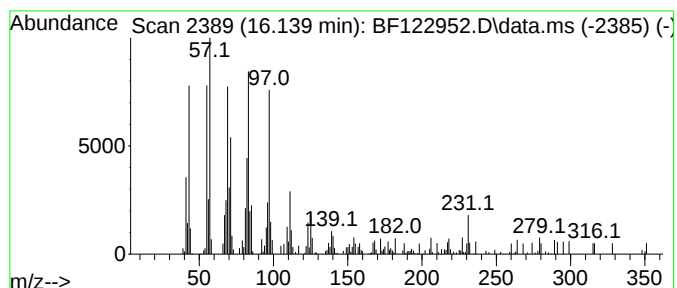
Instrument :
BNA_F
ClientSampled :
TP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cycloeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.139	2.17 ng	169400	Perylene-d12	15.592	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	83
2	Behenic alcohol	326	C22H46O	000661-19-8	70
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
4	1-Octadecanol, methyl ether	284	C19H40O	1000333-92-7	62
5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122952.D
Acq On : 8 Jan 2021 21:06
Operator : JU/CG
Sample : M1044-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.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...	2.222	12.9	ng	732076	1	6.916	1131250	20.0
2-Pentanone, 4-...	5.140	7.0	ng	395808	1	6.916	1131250	20.0
n-Hexadecanoic ...	11.975	2.9	ng	207628	4	11.451	1422580	20.0
unknown12.439	12.439	3.2	ng	226562	4	11.451	1422580	20.0
5-Eicosene, (E)-	13.939	7.1	ng	550402	5	14.098	1544270	20.0
Squalene	14.969	2.4	ng	189073	6	15.592	1562830	20.0
Cycloeicosane	16.139	2.2	ng	169400	6	15.592	1562830	20.0