

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112922\
 Data File : BF131455.D
 Acq On : 29 Nov 2022 14:22
 Operator : CG\JU
 Sample : N5762-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.305	28	37	43	rVB	1093816	1454277	29.25%	3.838%
2	2.416	49	56	64	rVB	95751	126290	2.54%	0.333%
3	4.569	418	422	427	rBV	57120	59000	1.19%	0.156%
4	5.187	520	527	540	rVB	1574004	2347937	47.22%	6.196%
5	5.575	587	593	596	rBV	4011344	4486500	90.24%	11.840%
6	5.957	655	658	662	rVB	170633	141867	2.85%	0.374%
7	6.575	756	763	766	rBV	3756344	4453648	89.58%	11.754%
8	6.946	822	826	829	rBV	1043583	877562	17.65%	2.316%
9	7.510	916	922	925	rBV	2468492	2951846	59.37%	7.790%
10	8.234	1040	1045	1048	rBV	1223074	1171446	23.56%	3.092%
11	9.316	1222	1229	1232	rBV	4757485	4971920	100.00%	13.121%
12	9.998	1339	1345	1348	rBV	1600997	1379799	27.75%	3.641%
13	10.798	1473	1481	1484	rBV	3045230	3394131	68.27%	8.957%
14	11.498	1594	1600	1602	rBV	1560637	1415469	28.47%	3.736%
15	11.557	1607	1610	1614	rVB3	59437	51549	1.04%	0.136%
16	12.016	1682	1688	1692	rBV3	106101	130106	2.62%	0.343%
17	12.716	1803	1807	1810	rVB	118172	107183	2.16%	0.283%
18	12.945	1840	1846	1849	rBV	101172	104368	2.10%	0.275%
19	13.092	1866	1871	1874	rBV	4486276	4708838	94.71%	12.427%
20	13.657	1962	1967	1969	rBV2	51959	56392	1.13%	0.149%
21	13.986	2020	2023	2024	rBV	68051	59869	1.20%	0.158%
22	14.016	2024	2028	2041	rVB2	287956	676616	13.61%	1.786%
23	14.151	2047	2051	2054	rBV	1386254	1177363	23.68%	3.107%
24	14.245	2064	2067	2072	rVB	68215	72163	1.45%	0.190%
25	14.304	2074	2077	2081	rVV	58638	54364	1.09%	0.143%
26	14.616	2127	2130	2134	rBV	80089	76481	1.54%	0.202%
27	14.674	2136	2140	2150	rVB9	40269	90394	1.82%	0.239%
28	14.939	2182	2185	2189	rVB	51101	52923	1.06%	0.140%
29	15.221	2230	2233	2237	rBV2	36323	52878	1.06%	0.140%
30	15.304	2243	2247	2251	rBV	82393	105204	2.12%	0.278%
31	15.686	2306	2312	2325	rVB	718691	1033222	20.78%	2.727%
32	16.180	2393	2396	2401	rVB4	32775	50291	1.01%	0.133%

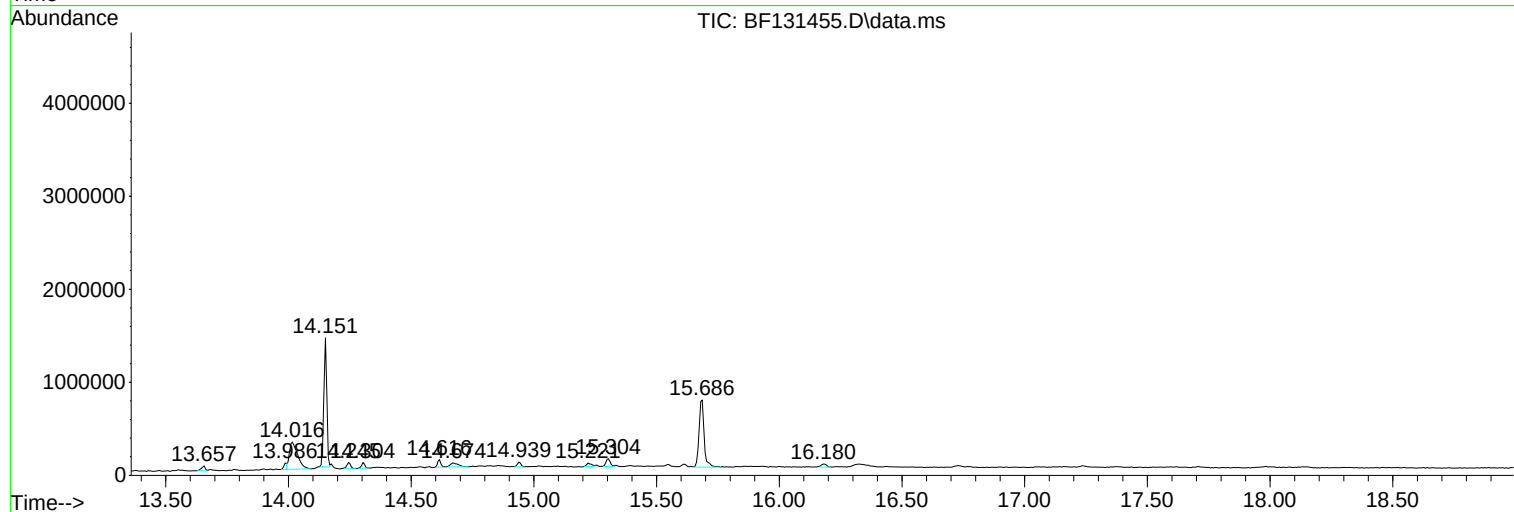
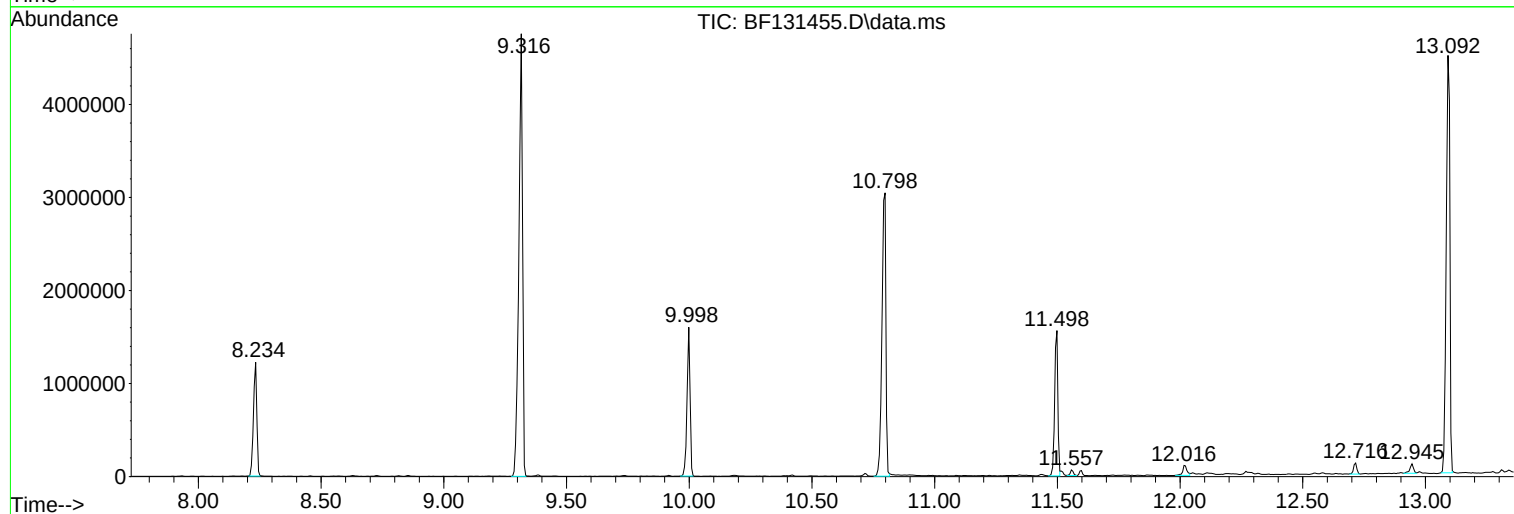
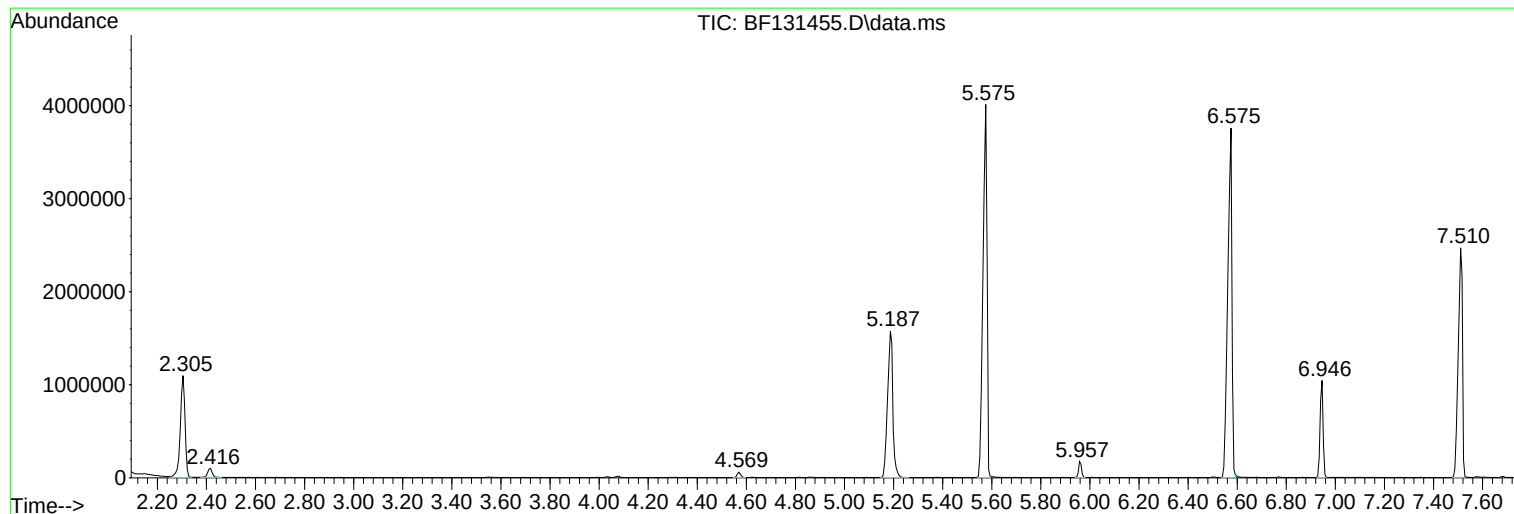
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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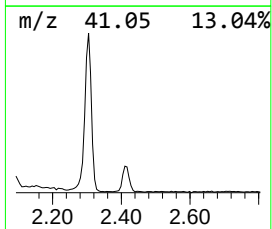
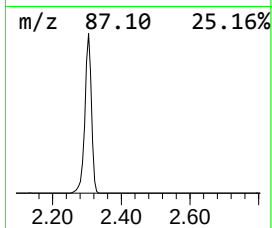
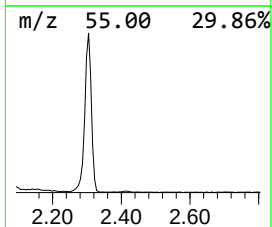
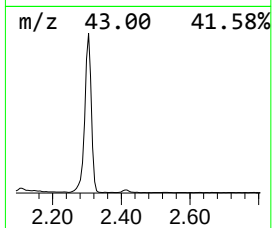
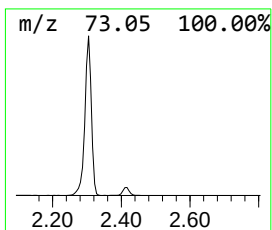
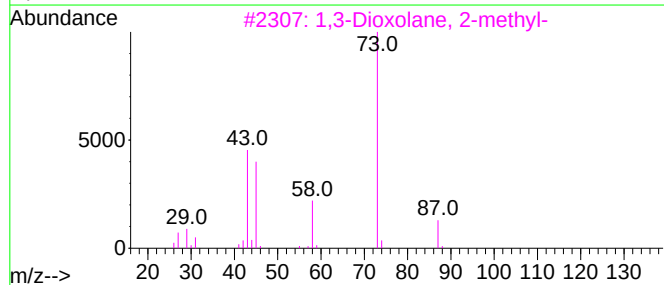
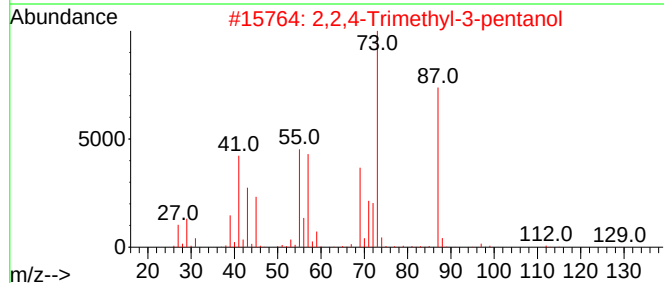
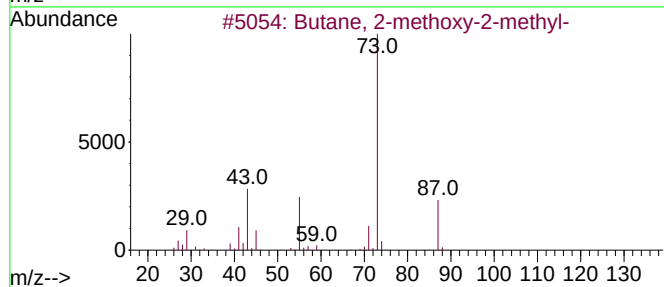
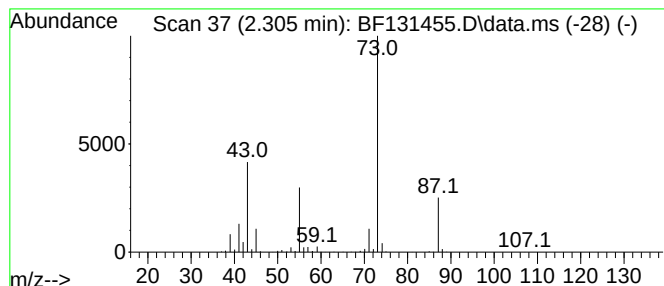
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	33.14 ng	1454280	1,4-Dichlorobenzene-d4	6.946

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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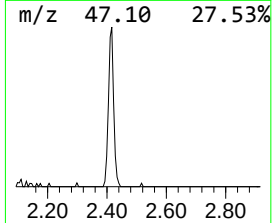
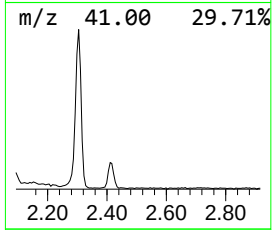
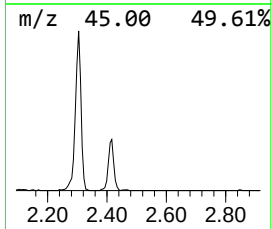
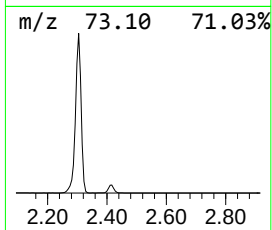
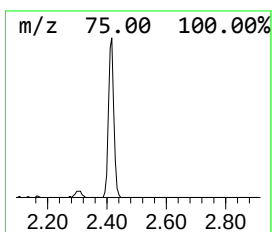
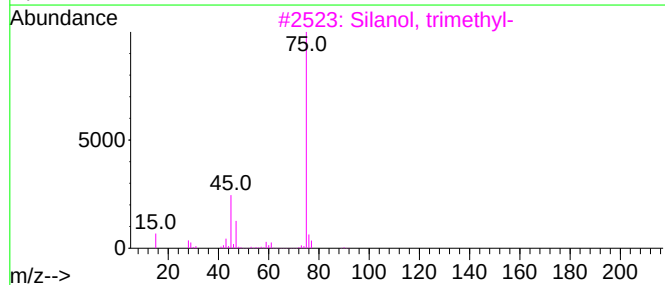
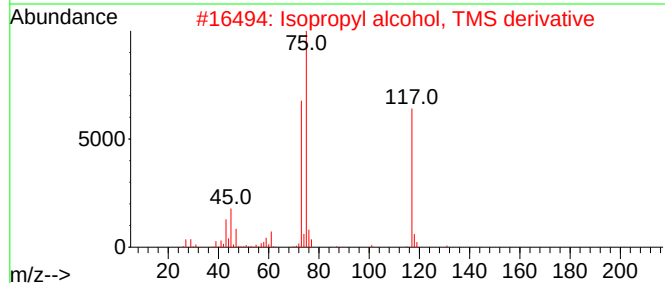
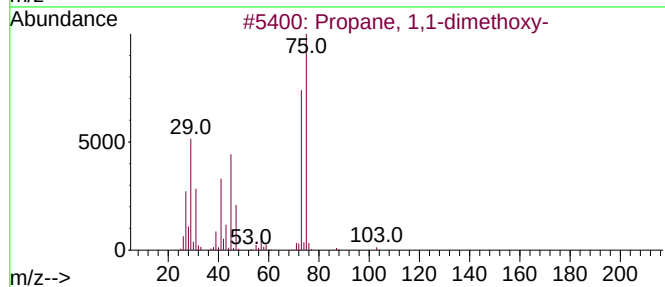
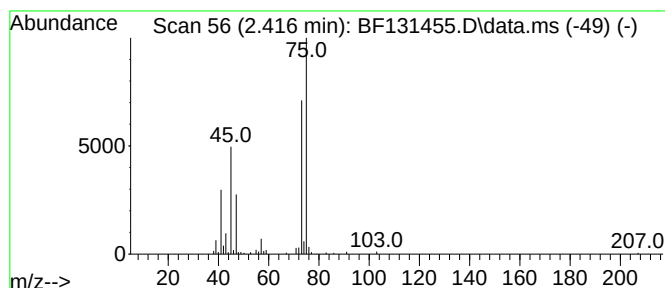
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.416	2.88 ng	126290	1,4-Dichlorobenzene-d4	6.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Isopropyl alcohol, TMS derivative	132	C6H16OSi	001825-64-5	83
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	40
4			Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	40
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	40



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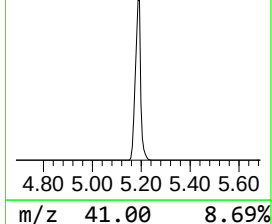
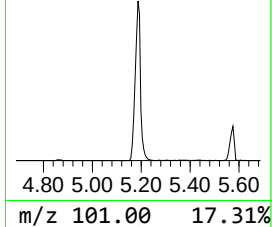
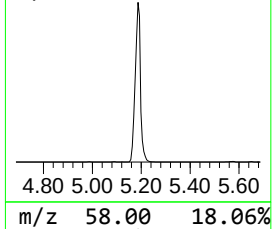
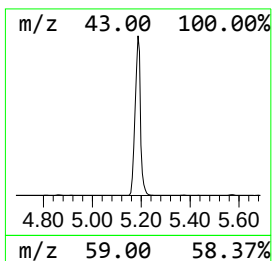
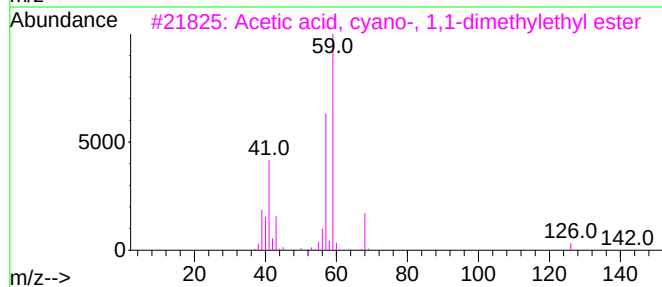
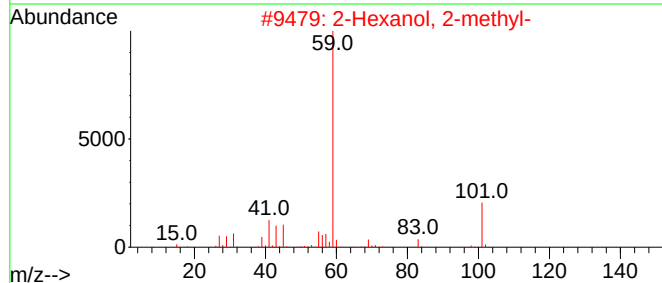
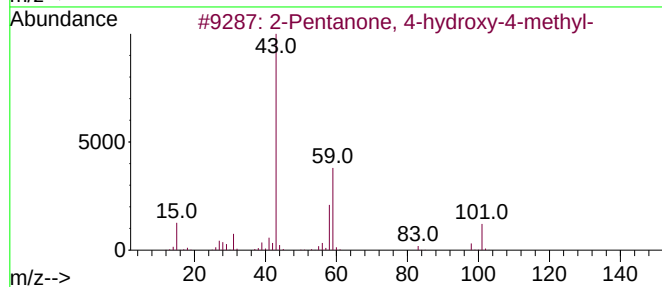
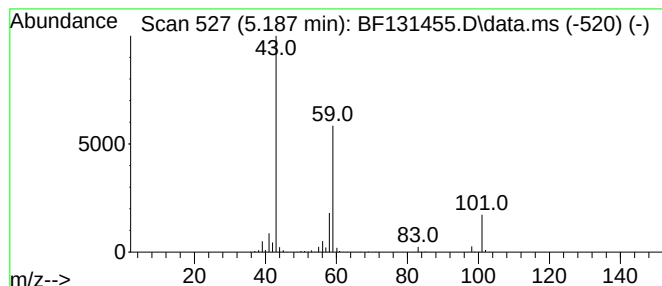
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	53.51 ng	2347940	1,4-Dichlorobenzene-d4	6.946

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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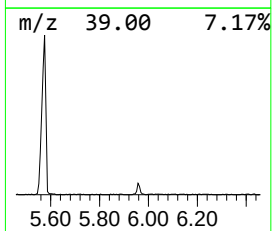
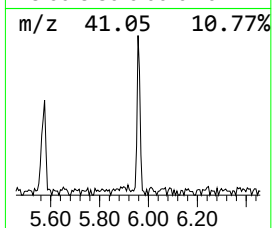
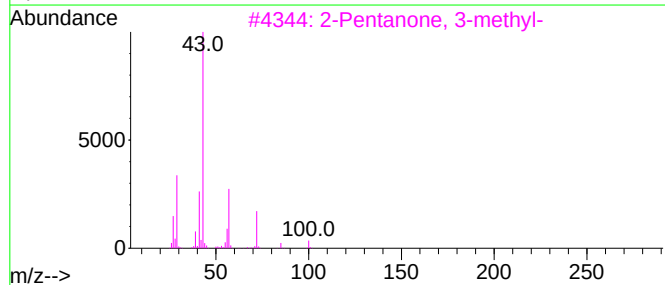
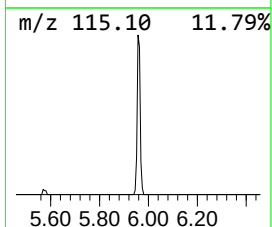
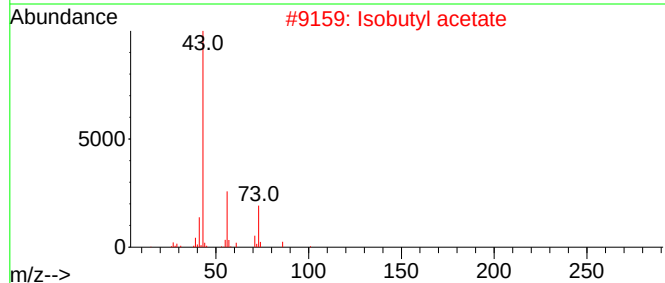
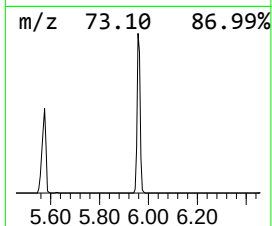
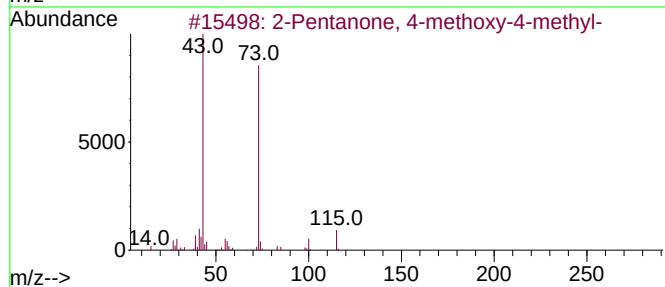
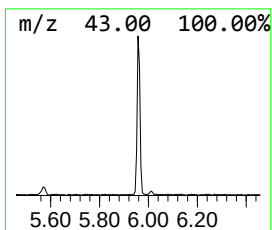
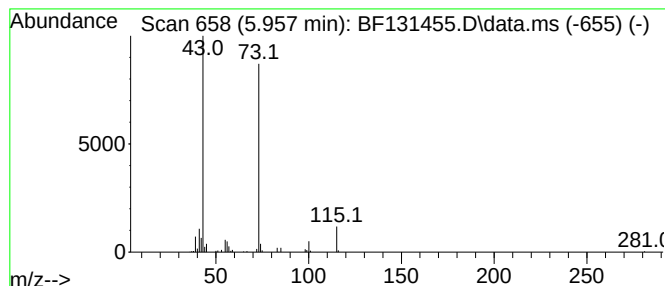
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.957	3.23 ng	141867	1,4-Dichlorobenzene-d4	6.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	23
3			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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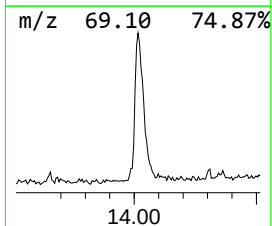
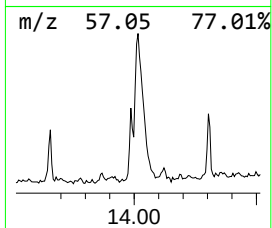
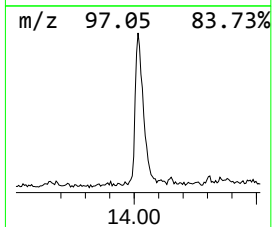
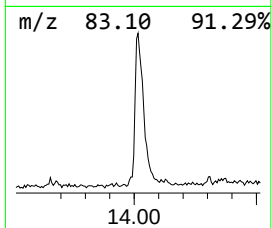
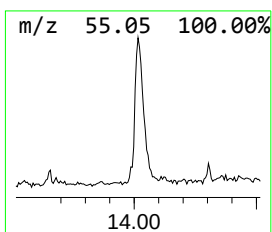
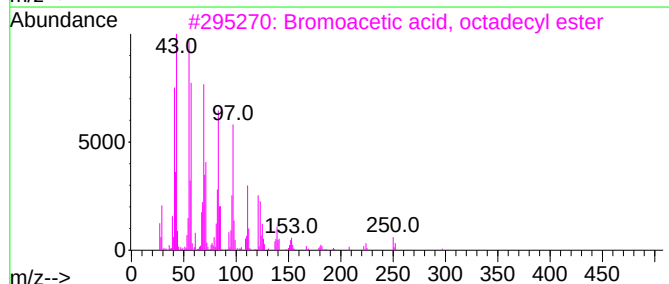
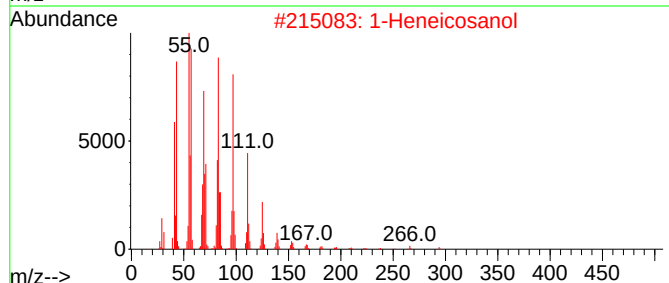
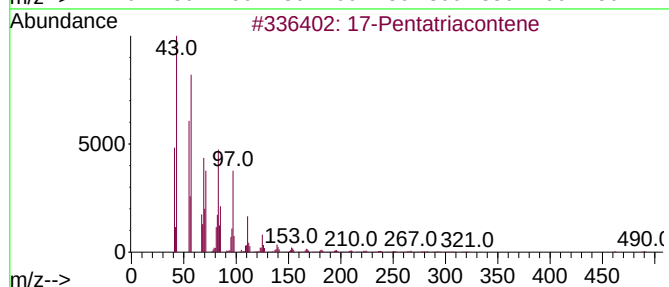
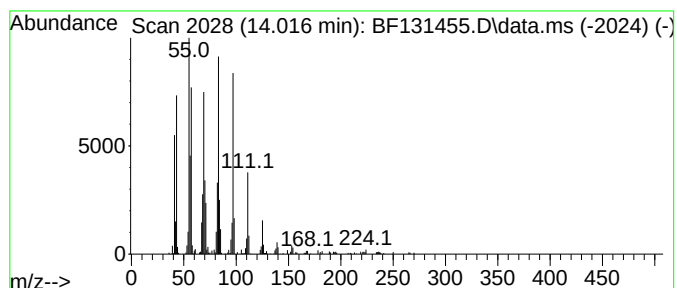
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	11.49 ng	676616	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
4			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	87
5			Behenic alcohol	326	C22H46O	000661-19-8	87



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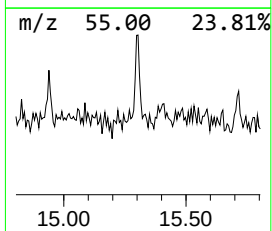
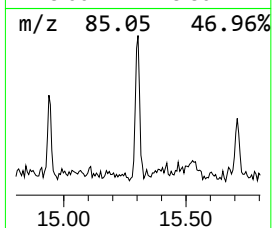
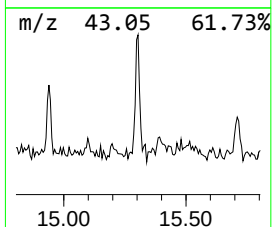
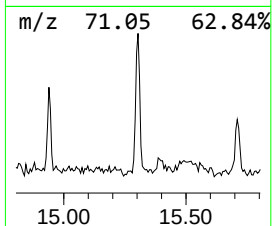
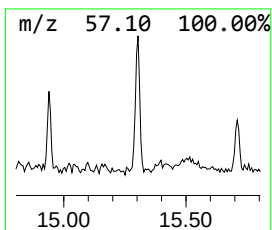
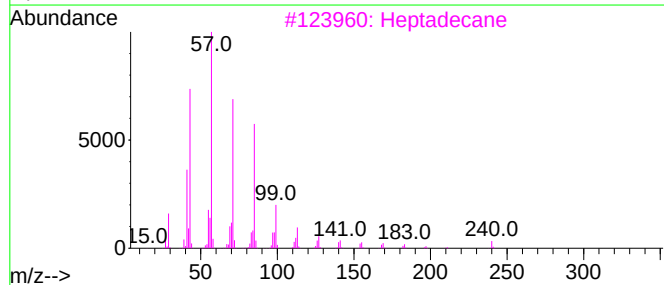
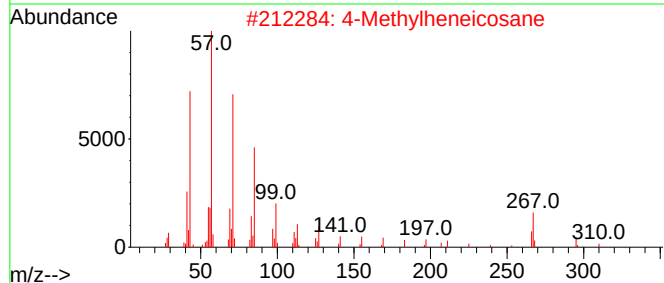
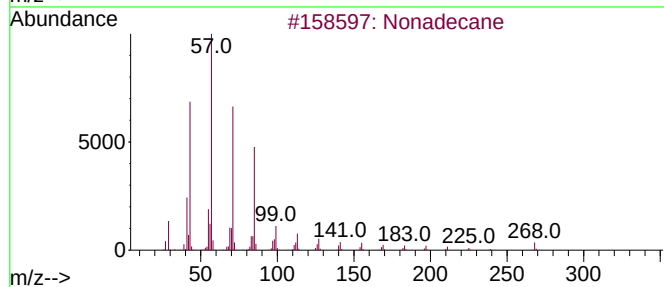
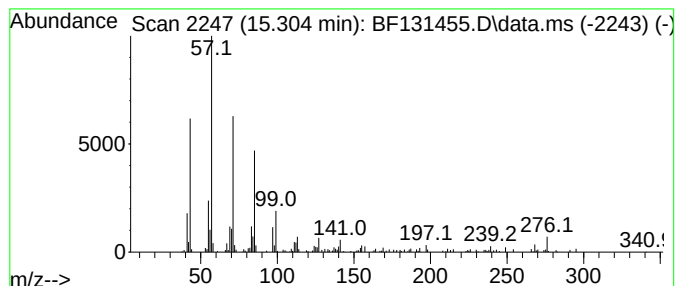
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	2.04 ng	105204	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			4-Methylheneicosane	310	C22H46	025117-29-7	87
3			Heptadecane	240	C17H36	000629-78-7	80
4			Octadecane	254	C18H38	000593-45-3	76
5			Heptacosane	380	C27H56	000593-49-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112922\
Data File : BF131455.D
Acq On : 29 Nov 2022 14:22
Operator : CG\JU
Sample : N5762-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.305	33.1	ng	1454280	1	6.946	877562	20.0
Propane, 1,1-di...	2.416	2.9	ng	126290	1	6.946	877562	20.0
2-Pentanone, 4-...	5.187	53.5	ng	2347940	1	6.946	877562	20.0
2-Pentanone, 4-...	5.957	3.2	ng	141867	1	6.946	877562	20.0
17-Pentatriacon...	14.016	11.5	ng	676616	5	14.151	1177360	20.0
Nonadecane	15.304	2.0	ng	105204	6	15.686	1033220	20.0