

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131133.D
 Acq On : 10 Nov 2022 20:39
 Operator : CG\JU
 Sample : N5520-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124042

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	7	13	19	rVB	618682	771414	44.65%	5.633%
2	2.269	27	31	38	rBV	35000	44759	2.59%	0.327%
3	4.487	404	408	415	rBV	75807	83747	4.85%	0.612%
4	5.110	509	514	524	rBV	539931	637939	36.93%	4.659%
5	5.510	577	582	585	rBV	1817244	1658463	96.00%	12.111%
6	5.904	644	649	652	rBV	29337	26222	1.52%	0.191%
7	6.516	748	753	756	rBV	1870401	1727630	100.00%	12.616%
8	6.887	812	816	820	rBV	626501	482634	27.94%	3.524%
9	7.451	907	912	915	rBV	1152092	1059828	61.35%	7.739%
10	8.169	1031	1034	1038	rBV	629332	573270	33.18%	4.186%
11	9.251	1213	1218	1221	rBV	1925700	1686295	97.61%	12.314%
12	9.851	1317	1320	1324	rVB	35386	28860	1.67%	0.211%
13	9.933	1330	1334	1337	rVB	680635	605508	35.05%	4.422%
14	10.351	1399	1405	1408	rBV	45322	41844	2.42%	0.306%
15	10.575	1438	1443	1445	rBV	18822	23720	1.37%	0.173%
16	10.722	1464	1468	1478	rVB	1095194	916657	53.06%	6.694%
17	10.828	1483	1486	1490	rBV	48644	52045	3.01%	0.380%
18	11.275	1559	1562	1565	rBV	34019	28378	1.64%	0.207%
19	11.304	1565	1567	1574	rVB2	21113	21796	1.26%	0.159%
20	11.422	1584	1587	1590	rBV	561917	506974	29.35%	3.702%
21	11.704	1632	1635	1638	rBV	32226	25301	1.46%	0.185%
22	12.116	1701	1705	1707	rBV	22257	19164	1.11%	0.140%
23	12.639	1791	1794	1798	rBV	39269	33276	1.93%	0.243%
24	12.874	1827	1834	1837	rBV2	41027	43477	2.52%	0.317%
25	13.010	1853	1857	1861	rBV	1252651	1072484	62.08%	7.832%
26	13.974	2014	2021	2030	rBV4	46875	155300	8.99%	1.134%
27	14.045	2030	2033	2034	rVV	60947	59946	3.47%	0.438%
28	14.074	2034	2038	2041	rVV	492769	480275	27.80%	3.507%
29	14.098	2041	2042	2047	rVV	33048	22120	1.28%	0.162%
30	14.168	2049	2054	2060	rVB	53783	61728	3.57%	0.451%
31	14.527	2112	2115	2120	rBV2	19034	20683	1.20%	0.151%
32	14.692	2140	2143	2149	rVB5	15682	18775	1.09%	0.137%
33	14.839	2166	2168	2173	rVB4	14754	19450	1.13%	0.142%
34	14.921	2178	2182	2186	rVV	56154	55279	3.20%	0.404%
35	15.127	2213	2217	2220	rBV	26753	39213	2.27%	0.286%
36	15.186	2224	2227	2233	rVB4	17063	23014	1.33%	0.168%

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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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.439	2267	2270	2274	rVB2	17644	21743	1.26%	0.159%
38	15.498	2278	2280	2287	rVV2	19403	24781	1.43%	0.181%
39	15.568	2287	2292	2303	rVV	376099	473354	27.40%	3.457%
40	16.027	2366	2370	2375	rVB4	14838	23904	1.38%	0.175%
41	17.074	2543	2548	2556	rBV5	9344	22632	1.31%	0.165%

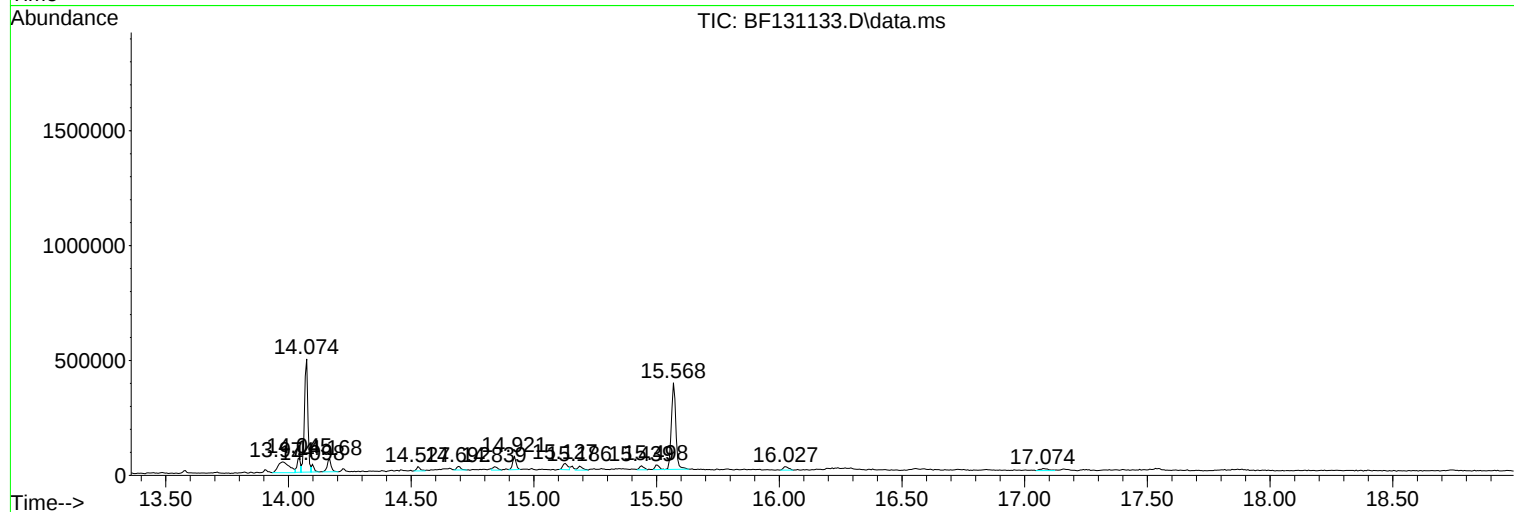
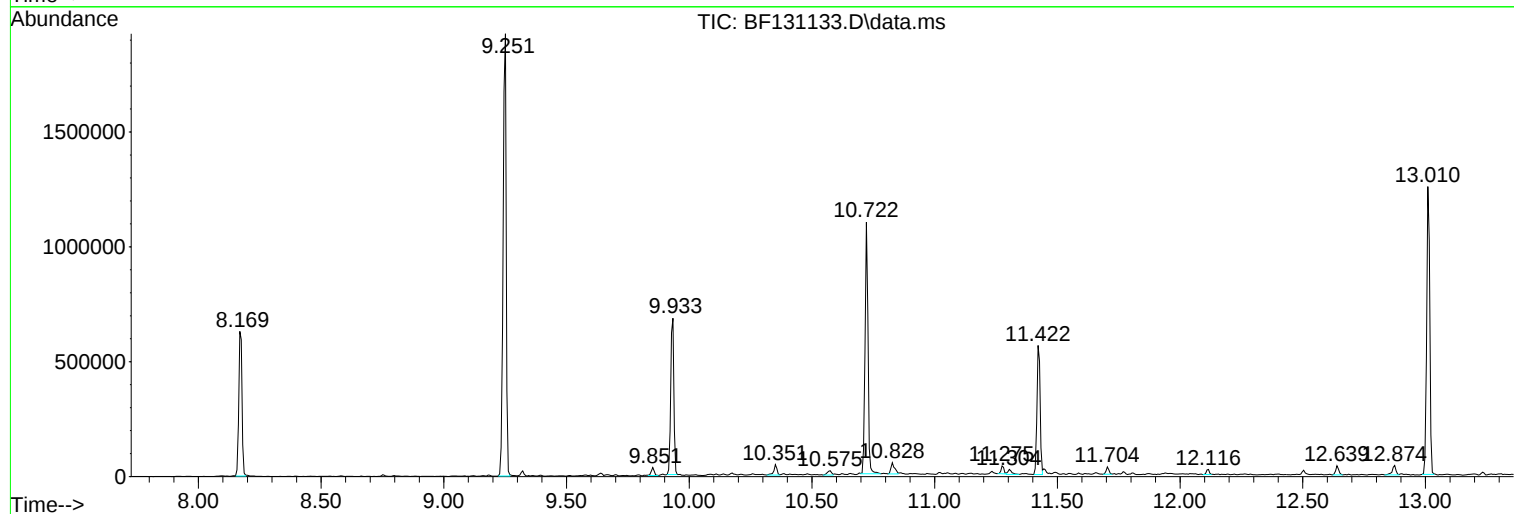
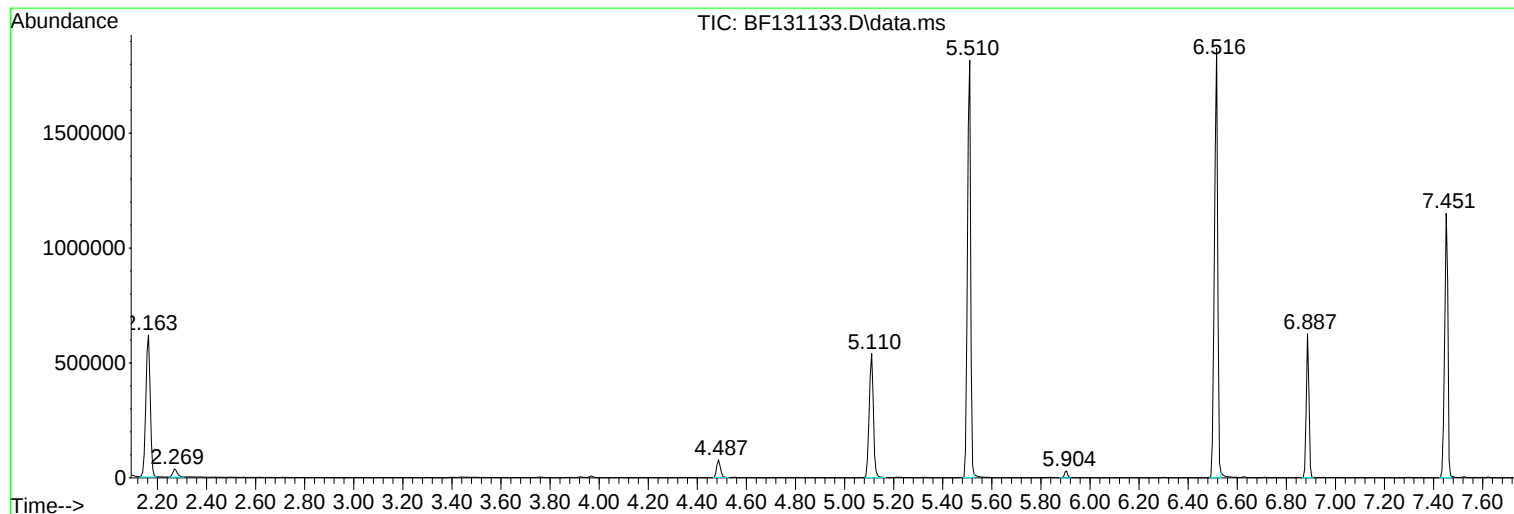
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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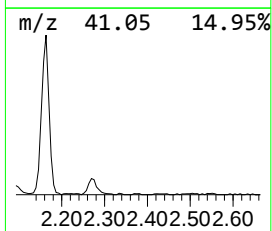
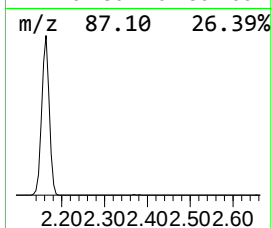
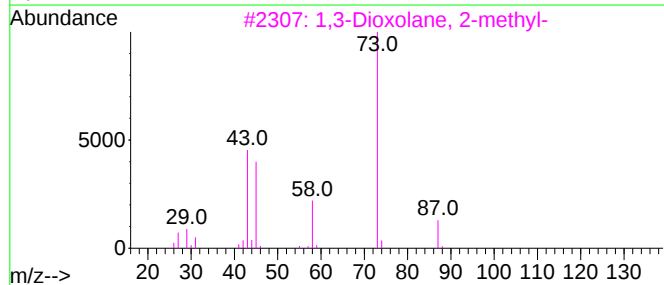
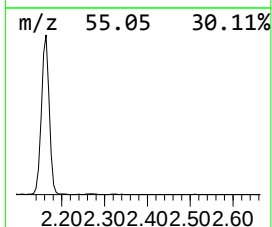
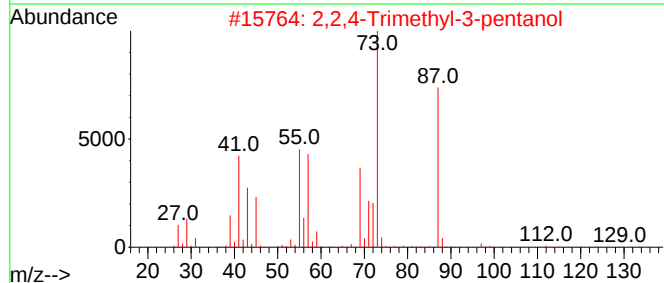
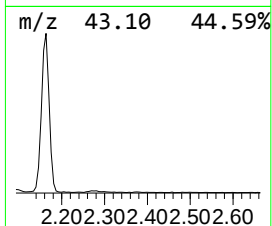
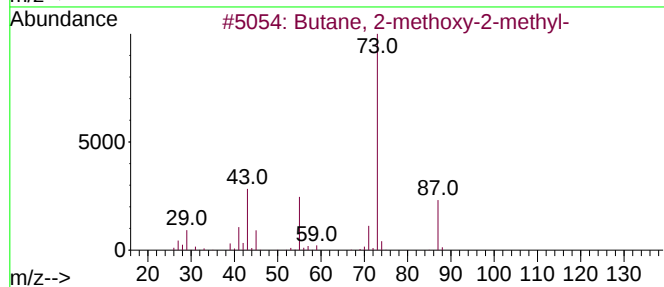
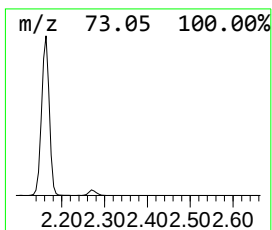
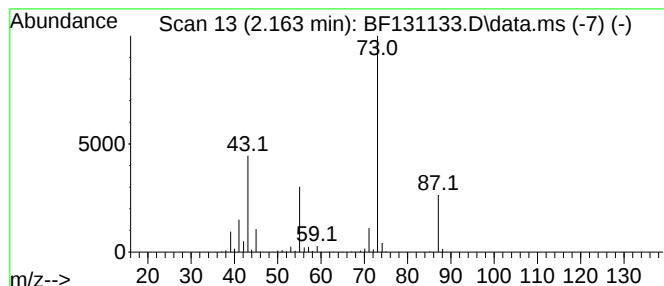
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	31.97 ng	771414	1,4-Dichlorobenzene-d4	6.887

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	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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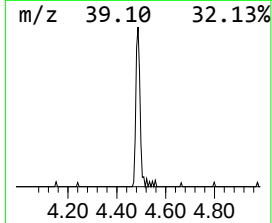
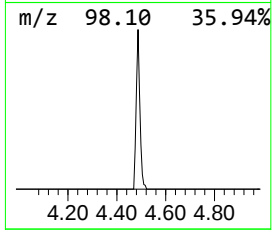
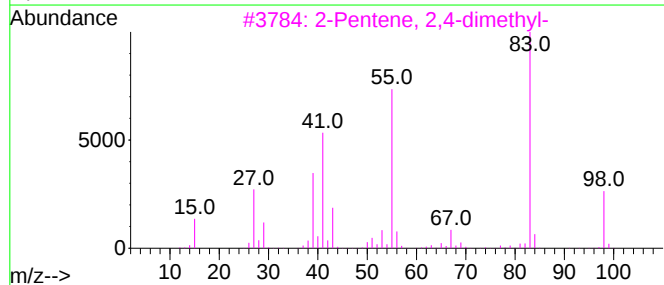
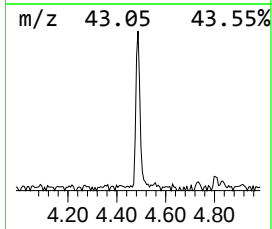
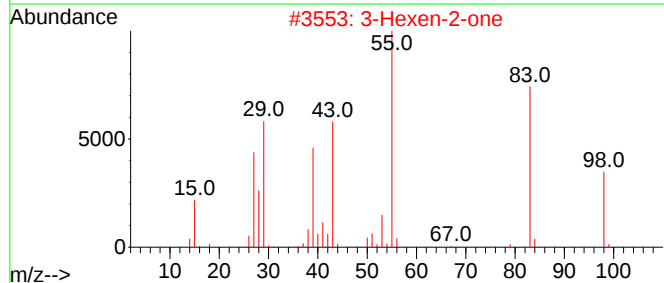
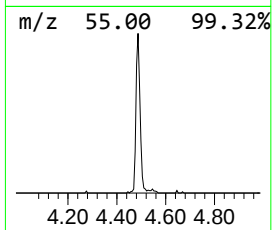
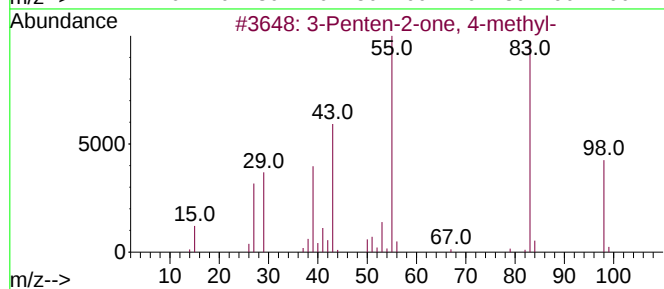
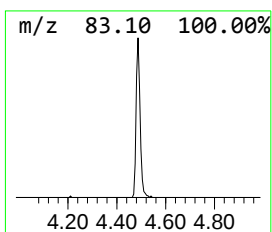
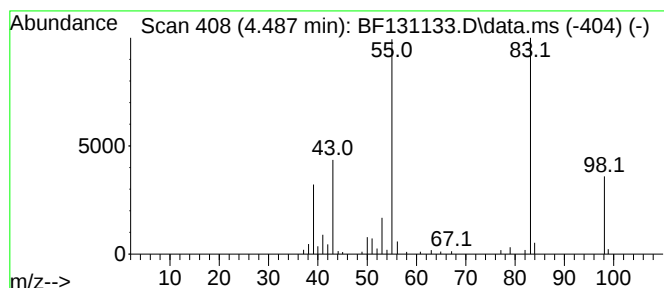
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	3.47 ng	83747	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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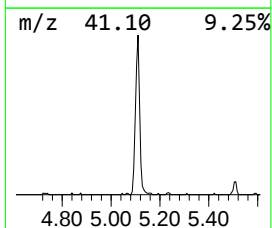
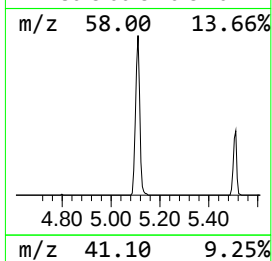
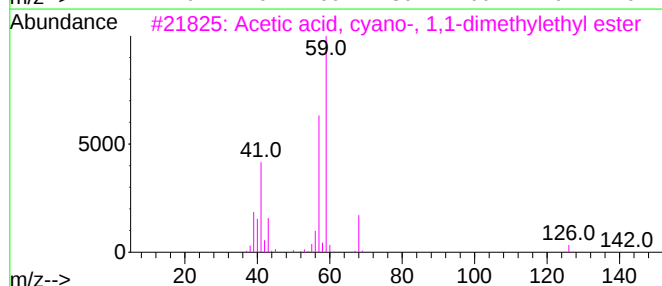
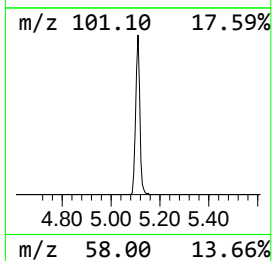
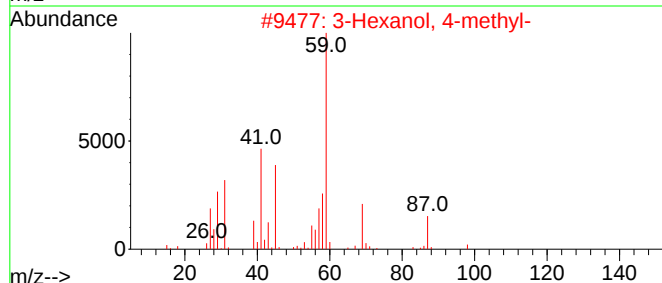
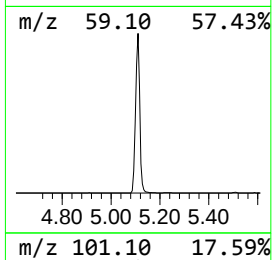
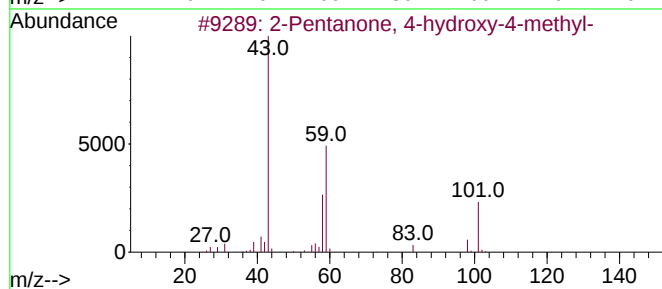
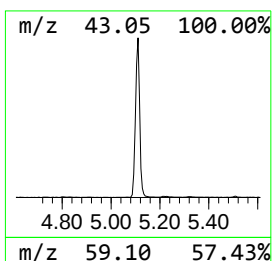
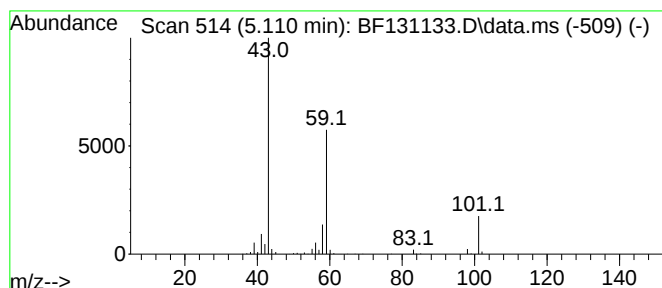
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.110	26.44 ng	637939	1,4-Dichlorobenzene-d4	6.887	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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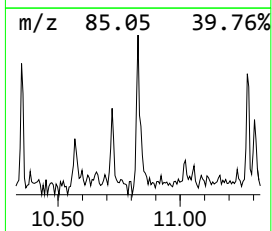
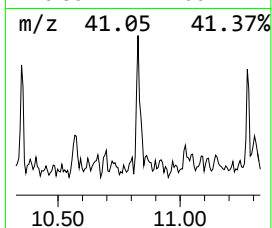
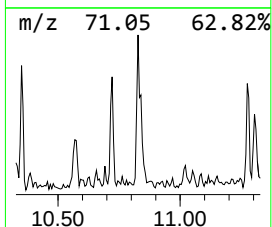
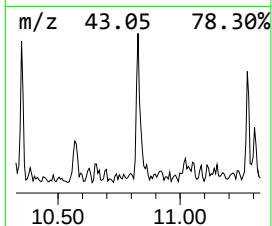
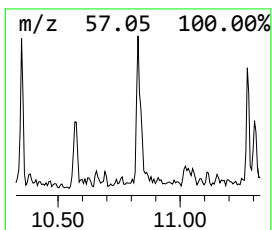
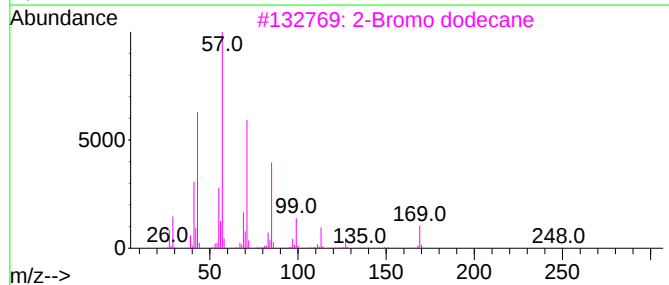
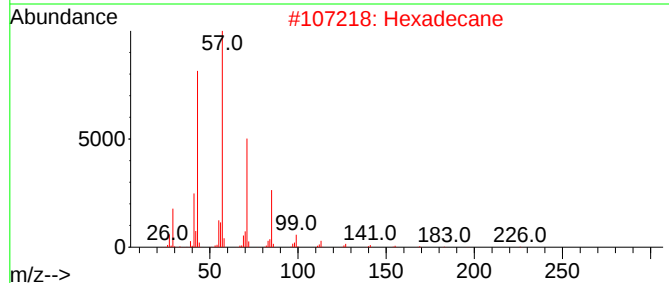
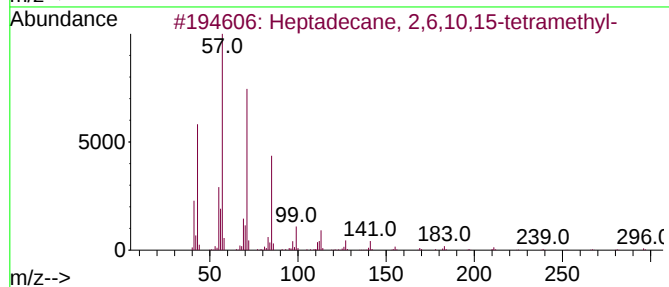
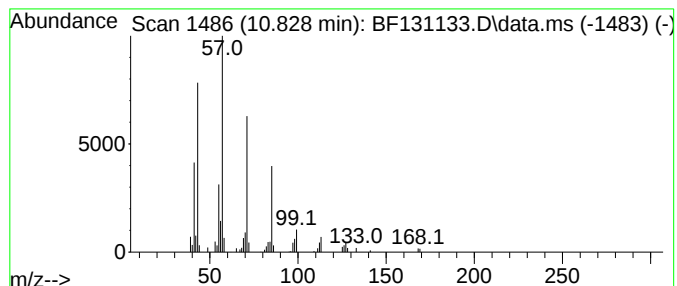
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.828	2.05 ng	52045	Phenanthrene-d10		11.422	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	86



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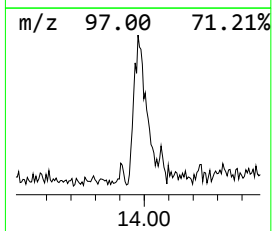
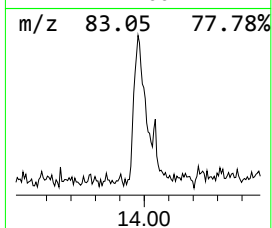
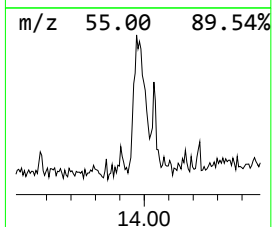
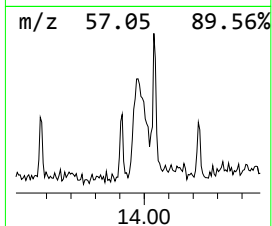
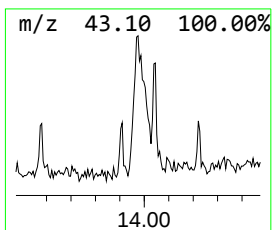
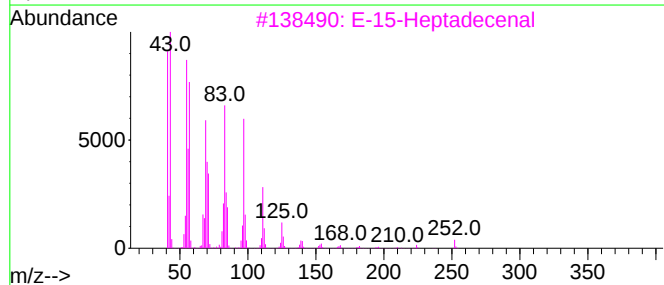
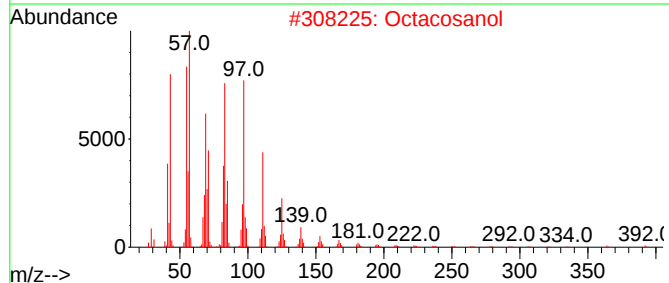
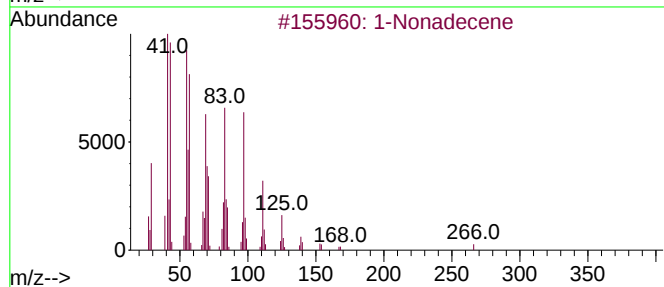
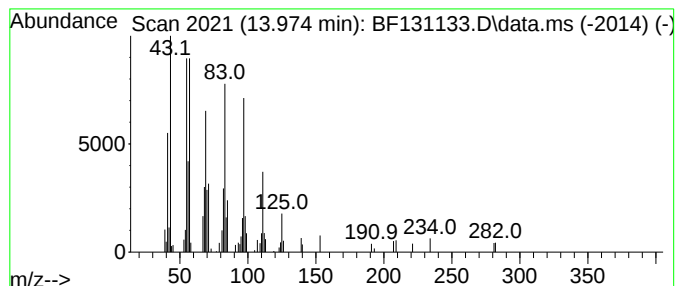
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	6.47 ng	155300	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	90
2			Octacosanol	410	C28H58O	000557-61-9	87
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	87
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5			Behenic alcohol	326	C22H46O	000661-19-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131133.D
Acq On : 10 Nov 2022 20:39
Operator : CG\JU
Sample : N5520-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124042

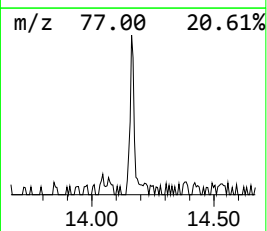
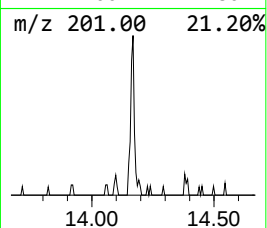
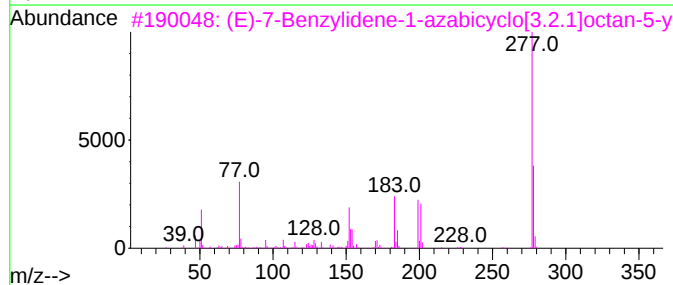
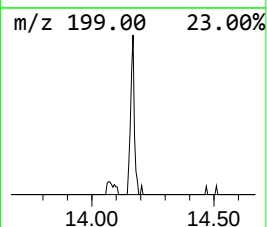
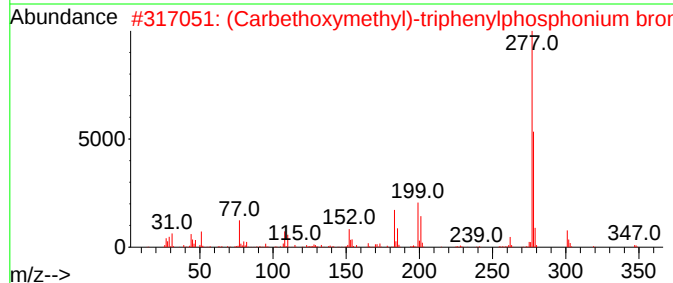
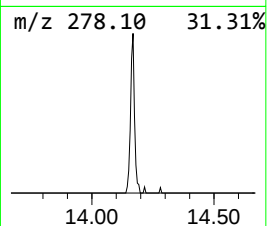
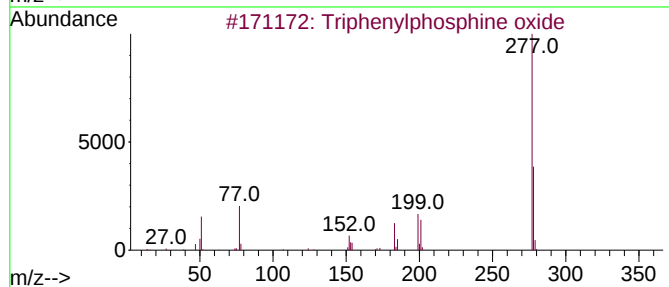
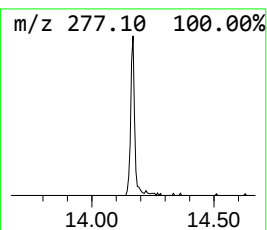
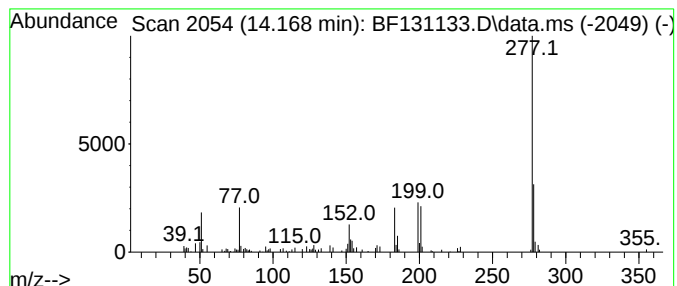
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	2.57 ng	61728	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	43
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
5			Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131133.D
Acq On : 10 Nov 2022 20:39
Operator : CG\JU
Sample : N5520-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

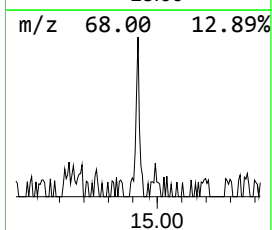
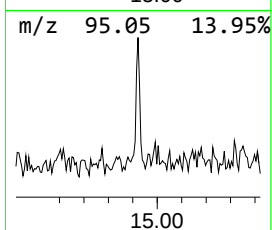
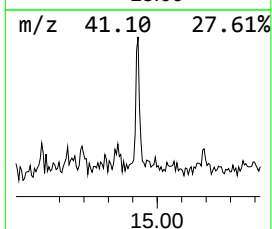
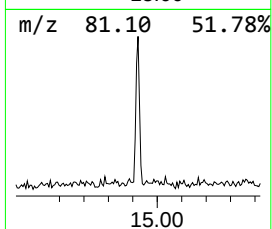
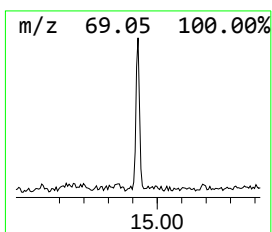
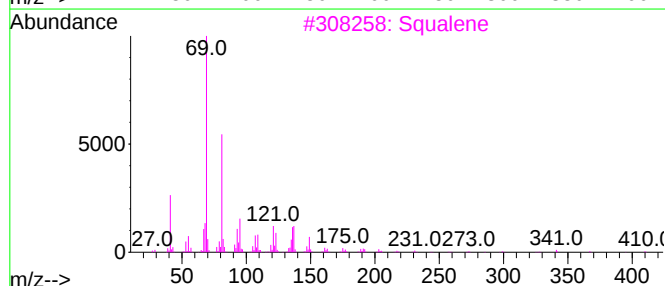
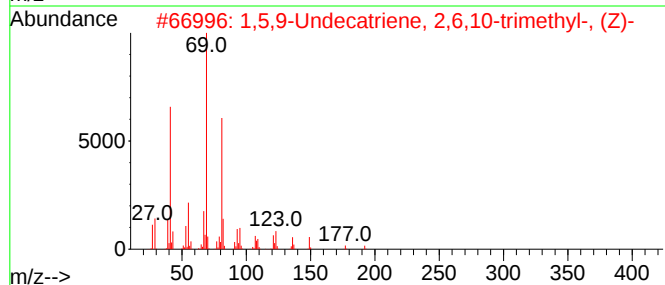
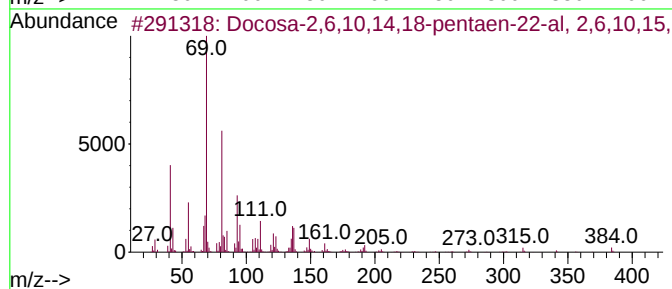
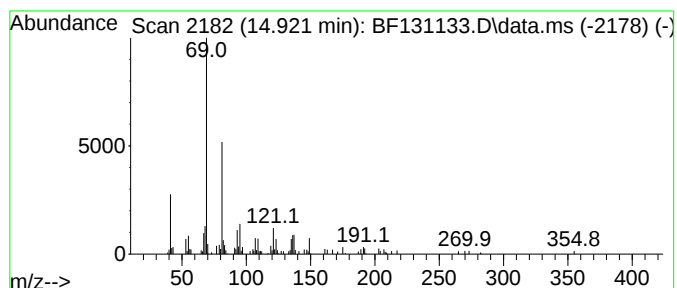
Instrument :
BNA_F
ClientSampleId :
124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosa-2,6,10,14,18-pentaen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.921	2.34 ng	55279	Perylene-d12	15.568	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	Squalene	410	C30H50	000111-02-4	87
4	Supraene	410	C30H50	007683-64-9	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131133.D
Acq On : 10 Nov 2022 20:39
Operator : CG\JU
Sample : N5520-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.163	32.0	ng	771414	1	6.887	482634	20.0
3-Penten-2-one,...	4.487	3.5	ng	83747	1	6.887	482634	20.0
2-Pentanone, 4-...	5.110	26.4	ng	637939	1	6.887	482634	20.0
Heptadecane, 2,...	10.828	2.0	ng	52045	4	11.422	506974	20.0
1-Nonadecene	13.974	6.5	ng	155300	5	14.074	480275	20.0
Triphenylphosph...	14.169	2.6	ng	61728	5	14.074	480275	20.0
Docosa-2,6,10,1...	14.921	2.3	ng	55279	6	15.568	473354	20.0