

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122220\
 Data File : BF122831.D
 Acq On : 23 Dec 2020 1:09
 Operator : JU/CG
 Sample : L5193-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LLEXSITUTV-024-001-SO

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-BF120520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	18	rVB	287025	384005	9.12%	1.483%
2	5.028	496	500	518	rVB	440739	538512	12.78%	2.080%
3	5.439	566	570	587	rBV	1941384	1812910	43.03%	7.003%
4	6.451	738	742	758	rBV	2319952	2239444	53.16%	8.650%
5	6.816	801	804	814	rBV	1192892	975234	23.15%	3.767%
6	7.380	895	900	903	rBV	1896143	1833176	43.52%	7.081%
7	8.104	1018	1023	1047	rBV	1343890	1287508	30.56%	4.973%
8	9.180	1200	1206	1209	rBV	3543589	3504936	83.20%	13.539%
9	9.569	1269	1272	1281	rBV	114747	127236	3.02%	0.491%
10	9.857	1316	1321	1337	rBV	1595988	1503863	35.70%	5.809%
11	10.645	1451	1455	1470	rBV	1250259	1394042	33.09%	5.385%
12	11.345	1569	1574	1591	rBV	1663669	1614086	38.32%	6.235%
13	12.933	1839	1844	1847	rBV	4231836	4212645	100.00%	16.272%
14	13.874	1992	2004	2017	rBV3	99696	458042	10.87%	1.769%
15	13.986	2019	2023	2038	rVB	1599597	1600799	38.00%	6.183%
16	15.086	2206	2210	2215	rVB	68222	74091	1.76%	0.286%
17	15.445	2265	2271	2288	rBV	1045233	1541017	36.58%	5.952%
18	15.886	2341	2346	2351	rBV	129351	181763	4.31%	0.702%
19	16.380	2424	2430	2437	rBV	129459	209605	4.98%	0.810%
20	16.956	2522	2528	2538	rVB	84309	164223	3.90%	0.634%
21	17.639	2638	2644	2654	rVB2	57818	141555	3.36%	0.547%
22	18.456	2777	2783	2793	rVB2	32829	89941	2.14%	0.347%

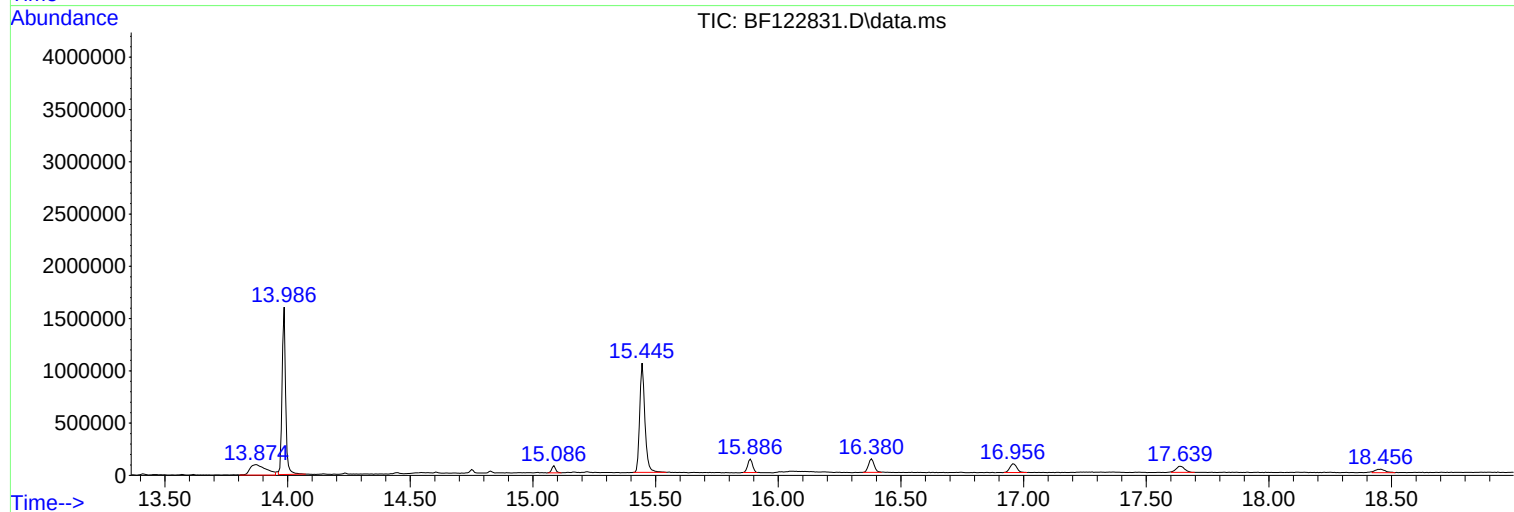
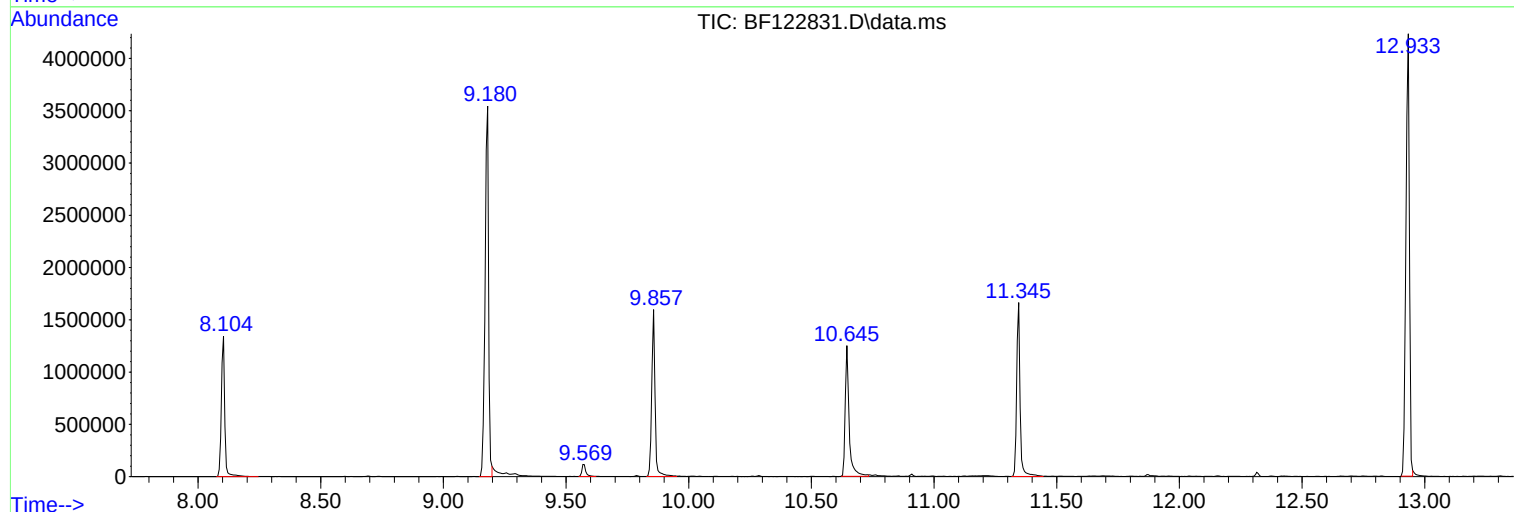
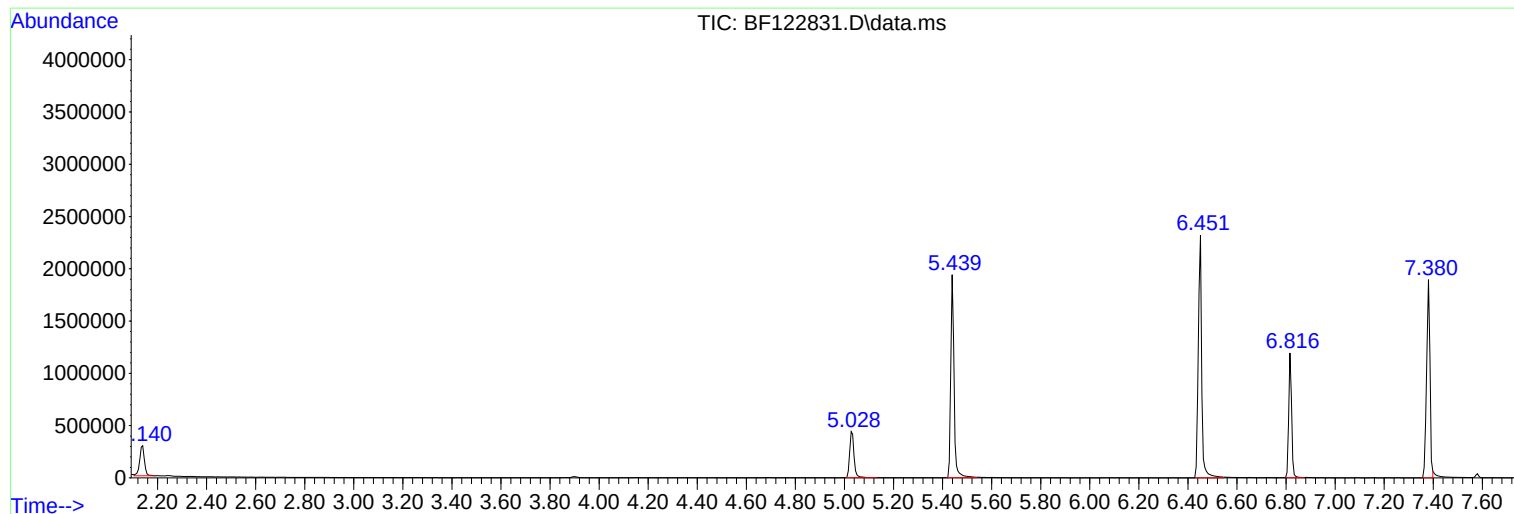
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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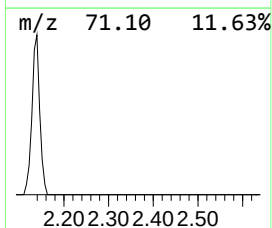
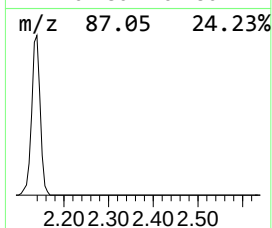
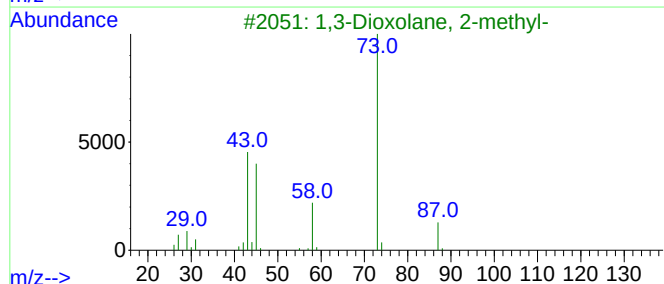
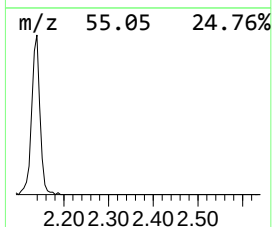
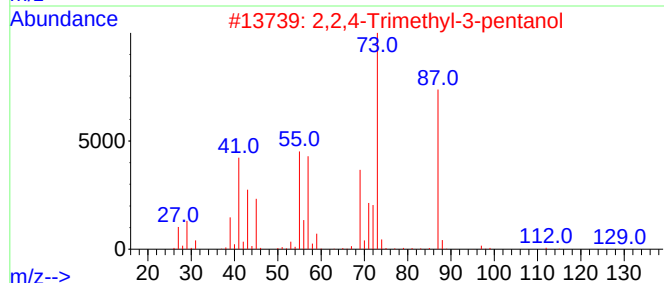
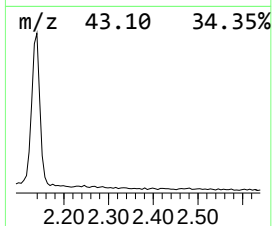
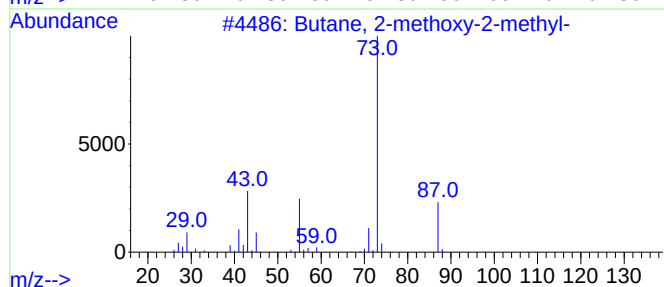
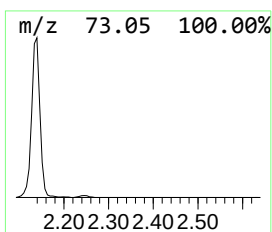
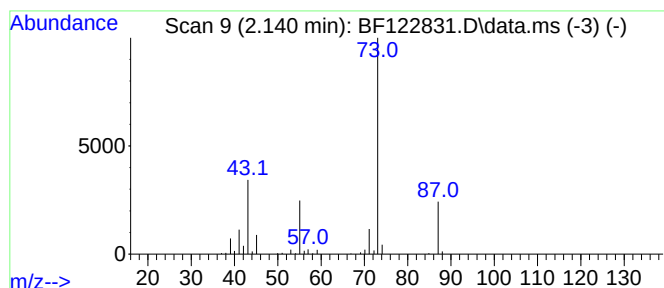
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	7.88 ng	384005	1,4-Dichlorobenzene-d4	6.816

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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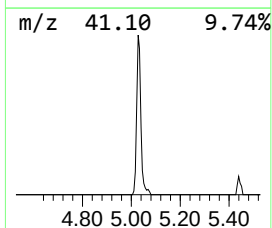
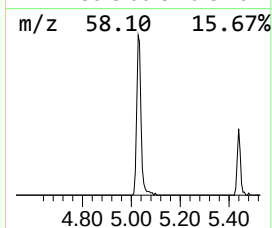
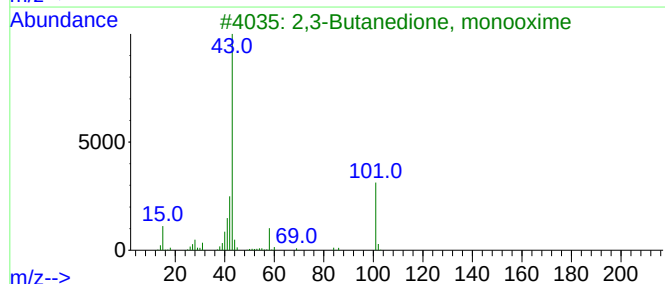
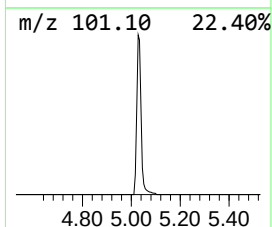
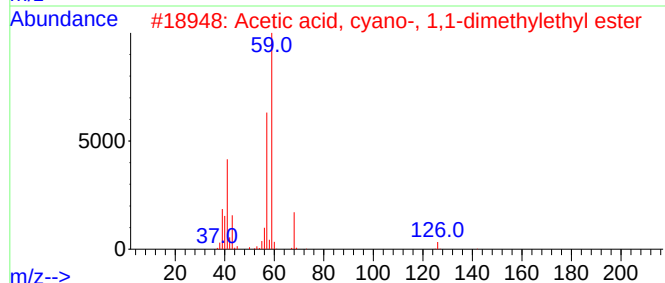
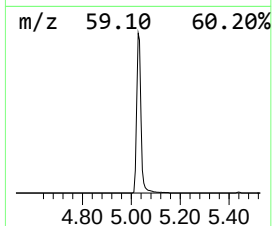
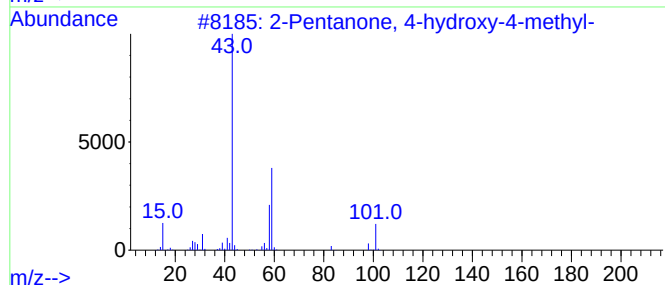
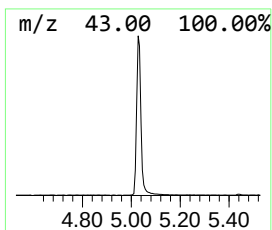
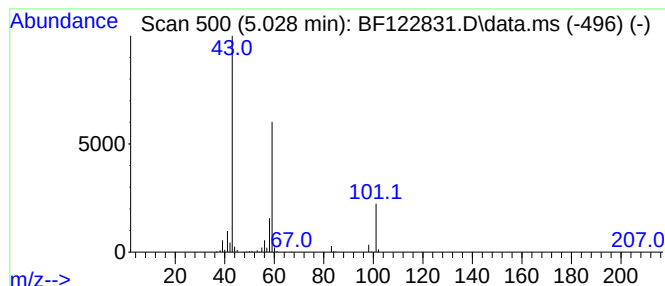
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.028	11.04 ng	538512	1,4-Dichlorobenzene-d4		6.816	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	17
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one		98	C6H10O	000109-49-9	9



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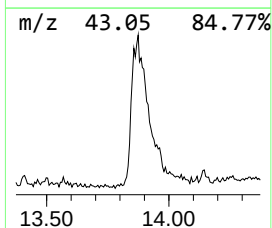
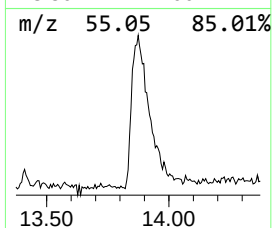
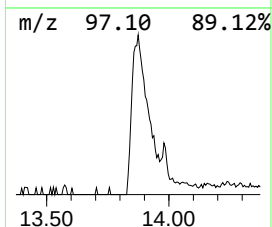
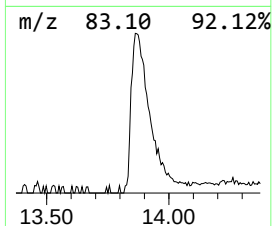
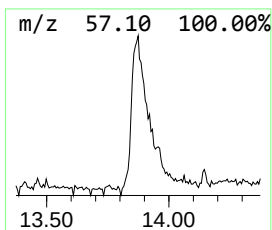
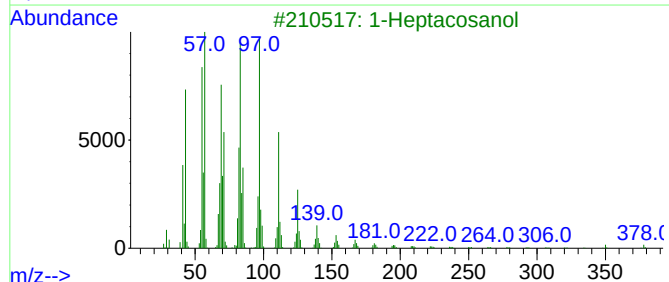
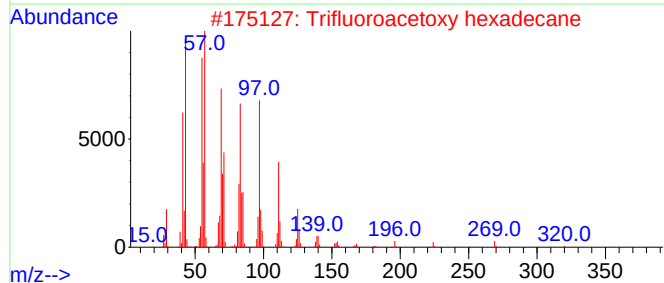
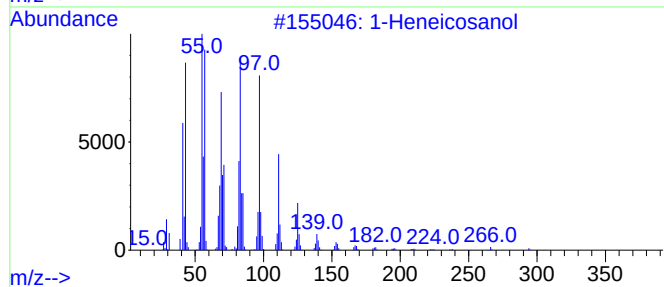
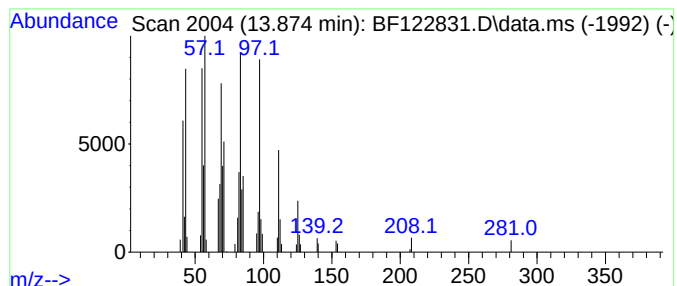
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Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.72 ng	458042	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	93
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



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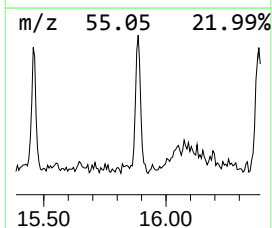
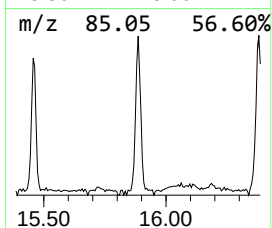
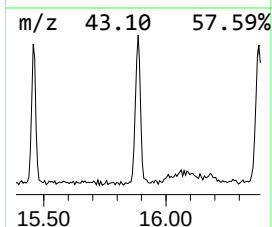
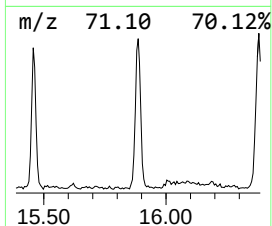
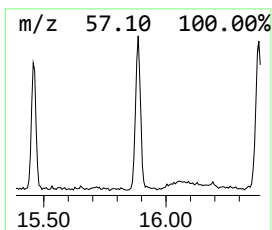
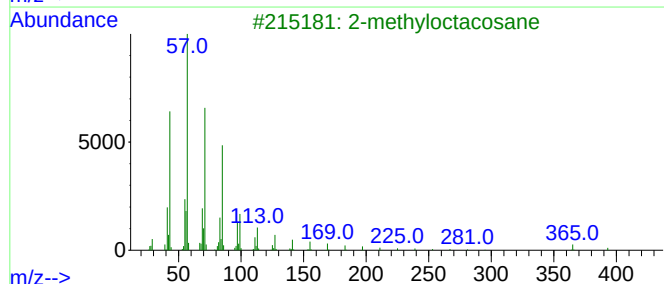
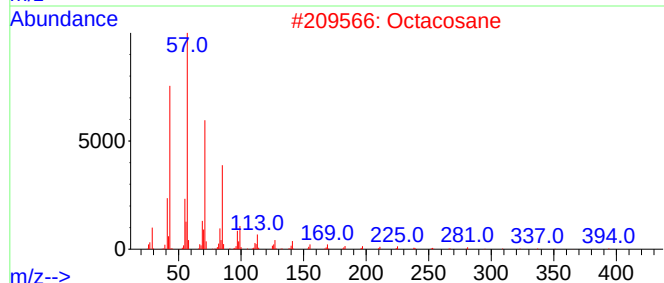
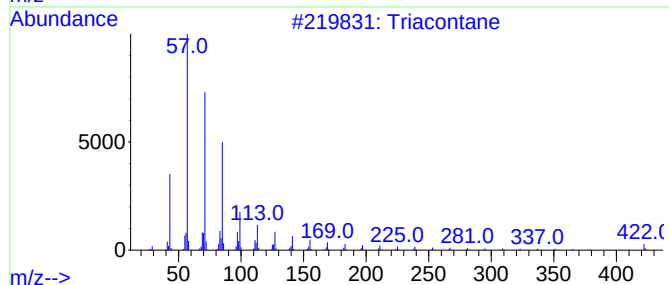
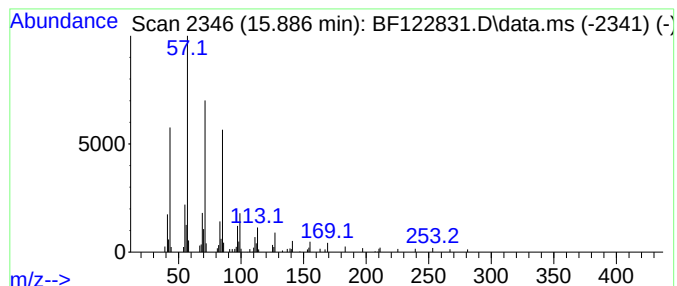
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.36 ng	181763	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	90



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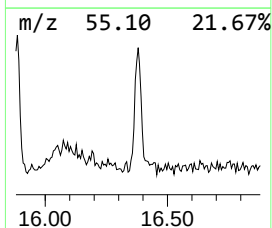
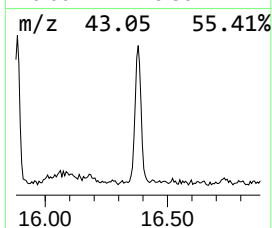
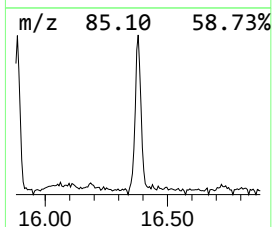
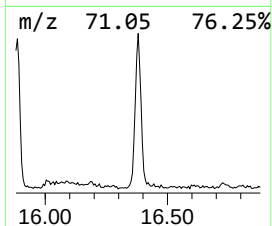
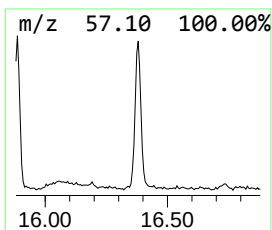
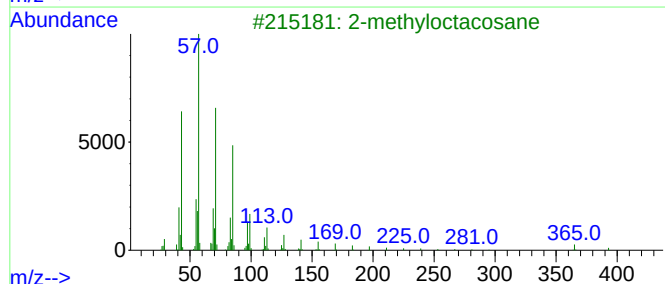
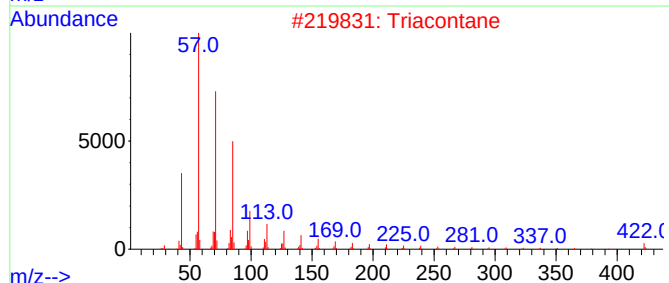
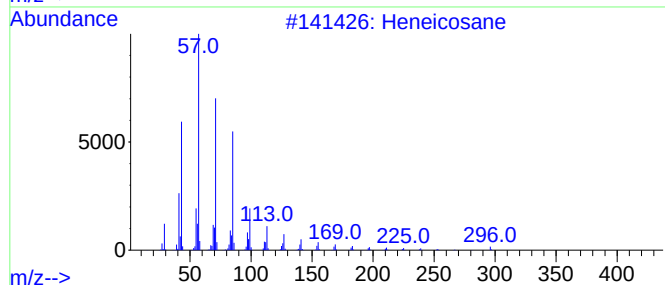
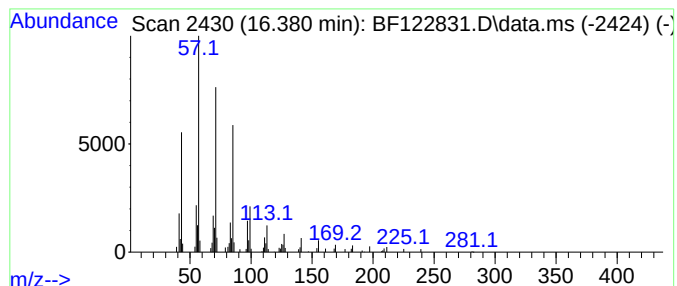
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.380	2.72 ng	209605	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Triacontane	422	C30H62	000638-68-6	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hexacosane	366	C26H54	000630-01-3	91



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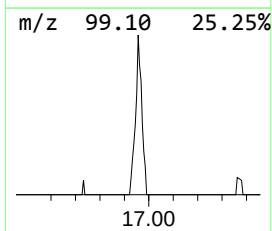
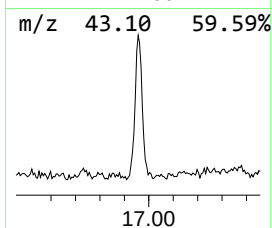
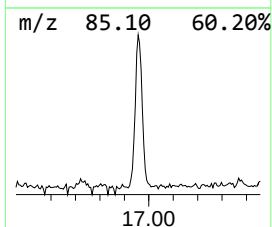
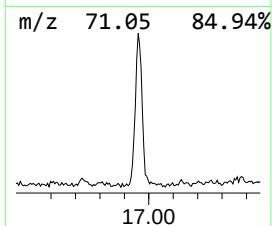
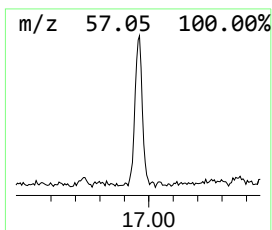
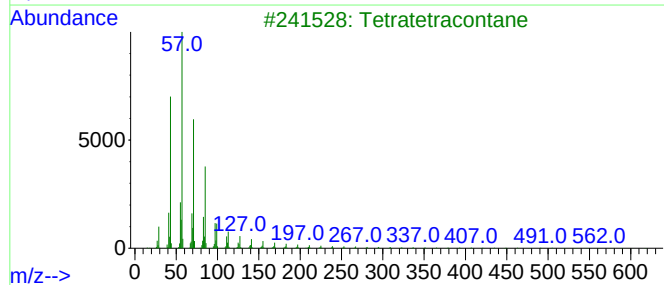
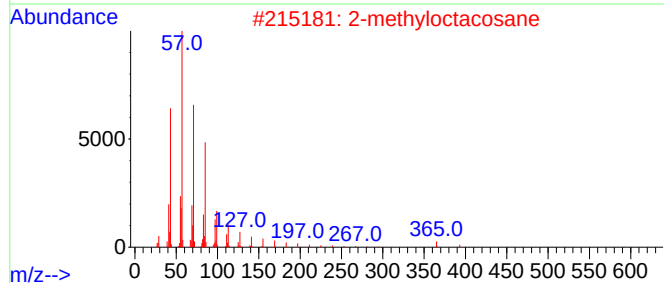
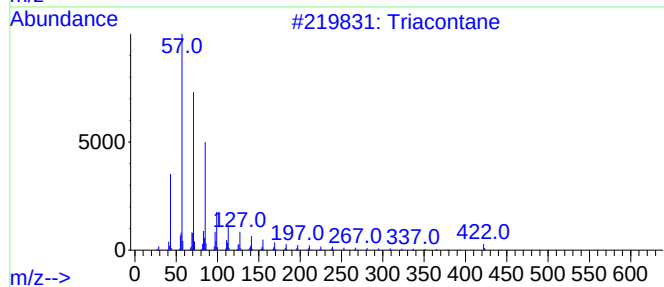
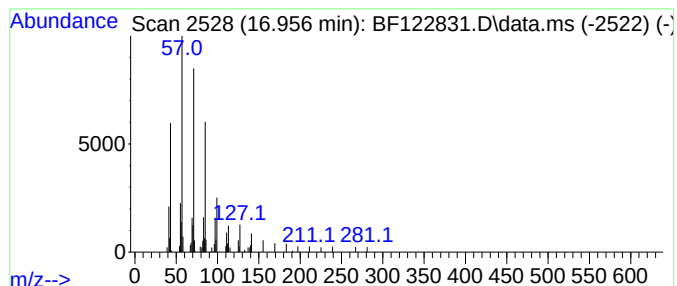
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.956	2.13 ng	164223	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122220\
Data File : BF122831.D
Acq On : 23 Dec 2020 1:09
Operator : JU/CG
Sample : L5193-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LLEXSITUTV-024-001-SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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...	2.140	7.9	ng	384005	1	6.816	975234	20.0
2-Pentanone, 4-...	5.028	11.0	ng	538512	1	6.816	975234	20.0
1-Heneicosanol	13.874	5.7	ng	458042	5	13.986	1600800	20.0
Triacontane	15.886	2.4	ng	181763	6	15.445	1541020	20.0
Heneicosane	16.380	2.7	ng	209605	6	15.445	1541020	20.0
2-methyloctacosane	16.956	2.1	ng	164223	6	15.445	1541020	20.0