LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131048.D
Acq On : 07 Nov 2022 17:43
Operator : CG\JU
Sample : N5415-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-18

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-BF110722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	11	16	23	rVB	465751	594053	27.36%	3.777%
2	2.293	29	35	40	rBV	34017	46661	2.15%	0.297%
3	4.499	406	410	417	rVB	49804	56757	2.61%	0.361%
4	5.122	511	516	525	rVB	367938	410792	18.92%	2.612%
5	5.516	578	583	586	rBV	1833404	1674010	77.09%	10.643%
6	6.522	749	754	757	rBV	1759196	1923079	88.56%	12.226%
7	6.898	814	818	821	rBV	716356	562621	25.91%	3.577%
8	7.463	909	914	917	rBV	1410326	1231096	56.69%	7.827%
9	8.181	1032	1036	1040	rBV	860745	745118	34.31%	4.737%
10	9.263	1214	1220	1223	rBV	2554090	2171565	100.00%	13.806%
11	9.945	1332	1336	1339	rVB	976891	852557	39.26%	5.420%
12	10.733	1466	1470	1473	rBV	1582360	1264194	58.22%	8.037%
13	11.433	1585	1589	1593	rBV	1001736	855520	39.40%	5.439%
14	11.498	1597	1600	1604	rVB2	34361	29955	1.38%	0.190%
15	11.951	1671	1677	1681	rBV3	33793	38945	1.79%	0.248%
16	12.880	1830	1835	1838	rBV2	21541	31703	1.46%	0.202%
17	13.022	1855	1859	1863	rBV	1889285	1753342	80.74%	11.147%
18	13.922	2008	2012	2014	rBV	38407	40981	1.89%	0.261%
19	13.957	2014	2018	2030	rVB3	79380	184879	8.51%	1.175%
20	14.080	2036	2039	2042	rVB	527573	462863	21.31%	2.943%
21	14.174	2051	2055	2059	rVB	62481	66970	3.08%	0.426%
22	14.233	2062	2065	2070	rVB	43396	41645	1.92%	0.265%
23	14.539	2114	2117	2120	rBV	45928	46641	2.15%	0.297%
24	14.857	2168	2171	2174	rVB	38731	36403	1.68%	0.231%
25	14.933	2182	2184	2190	rVB	33528	37222	1.71%	0.237%
26	15.204	2227	2230	2234	rVB3	30609	34873	1.61%	0.222%
27	15.580	2289	2294	2302	rVB2	420416	534362	24.61%	3.397%

Sum of corrected areas: 15728807

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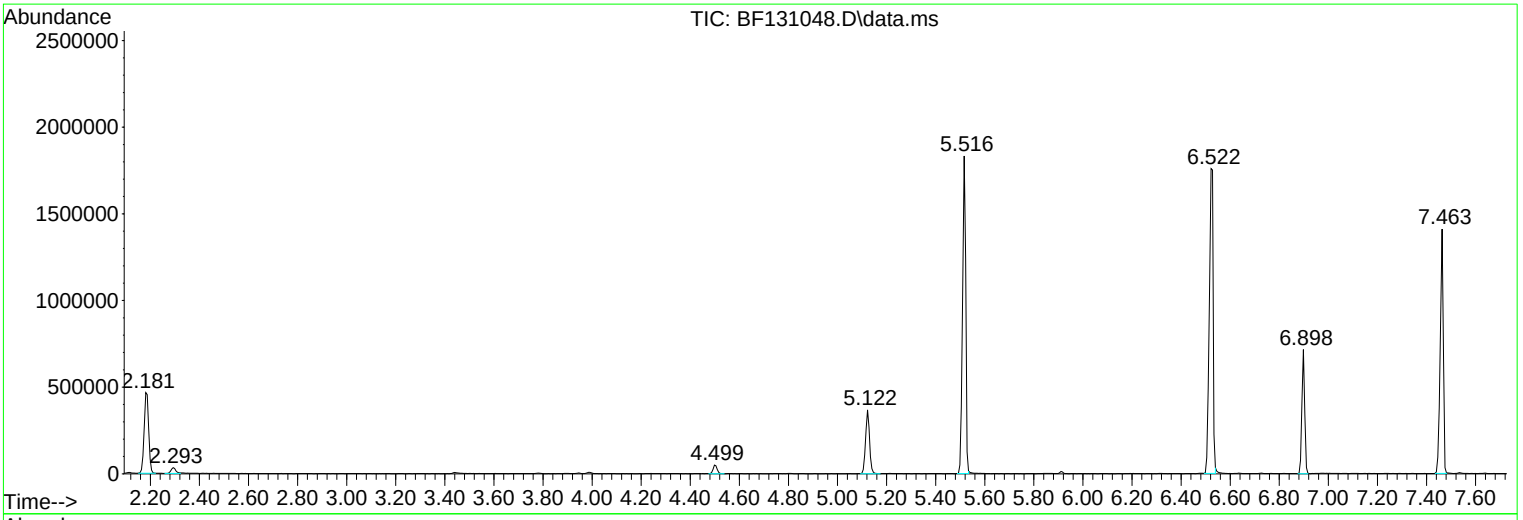
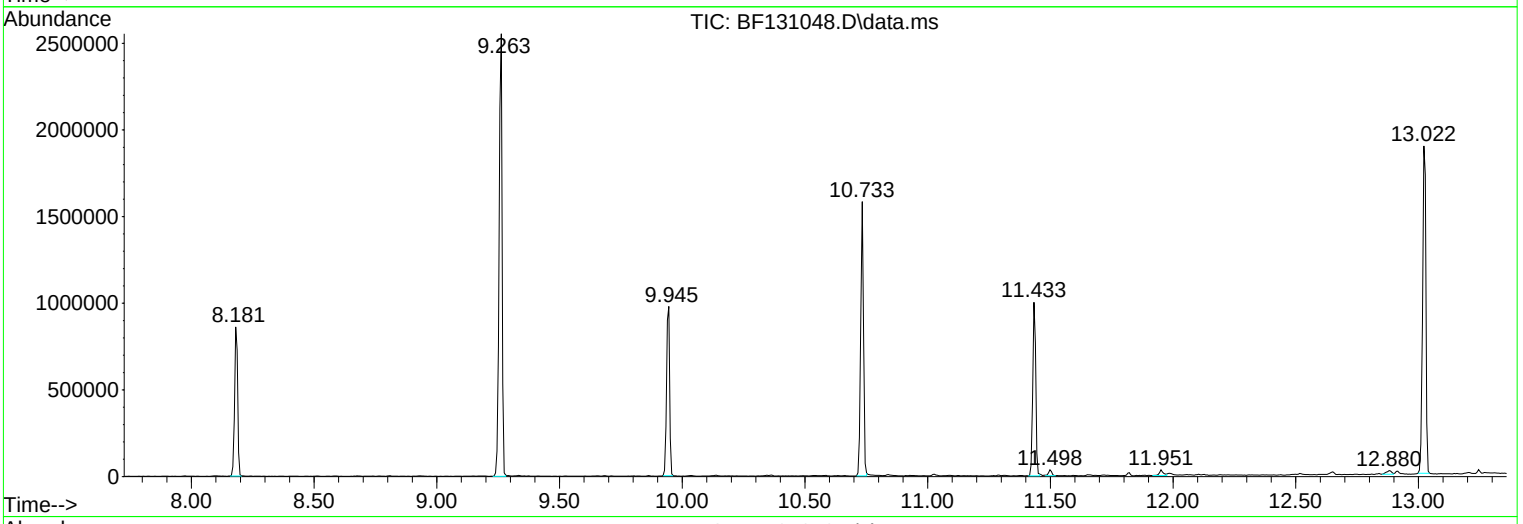
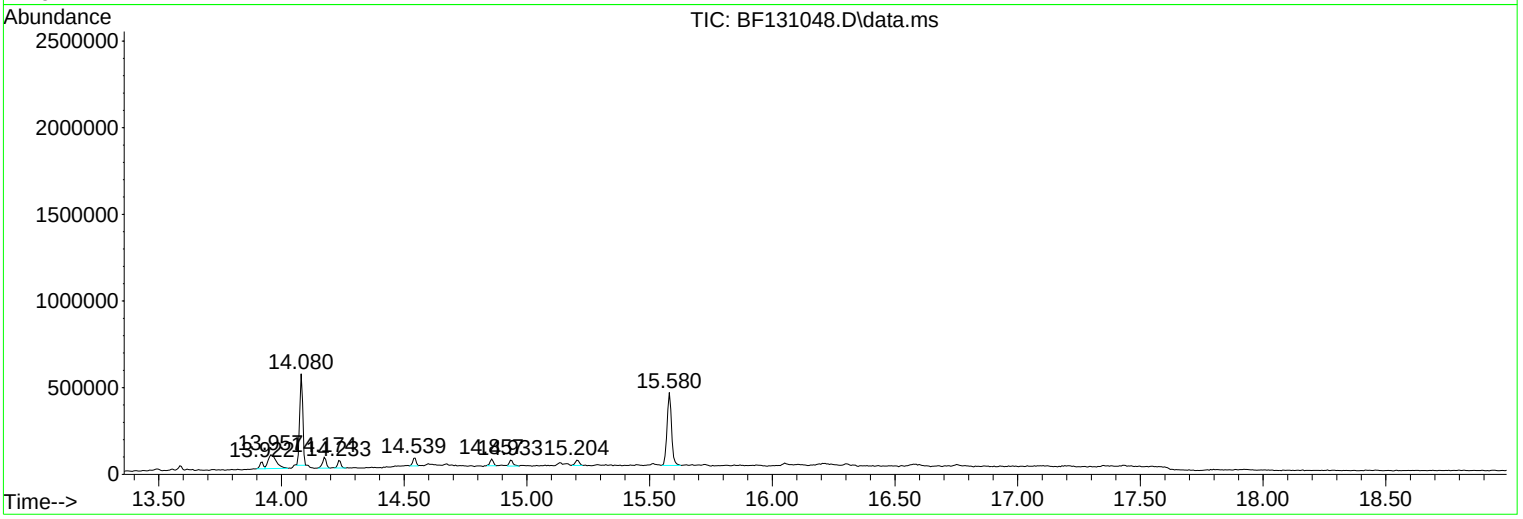
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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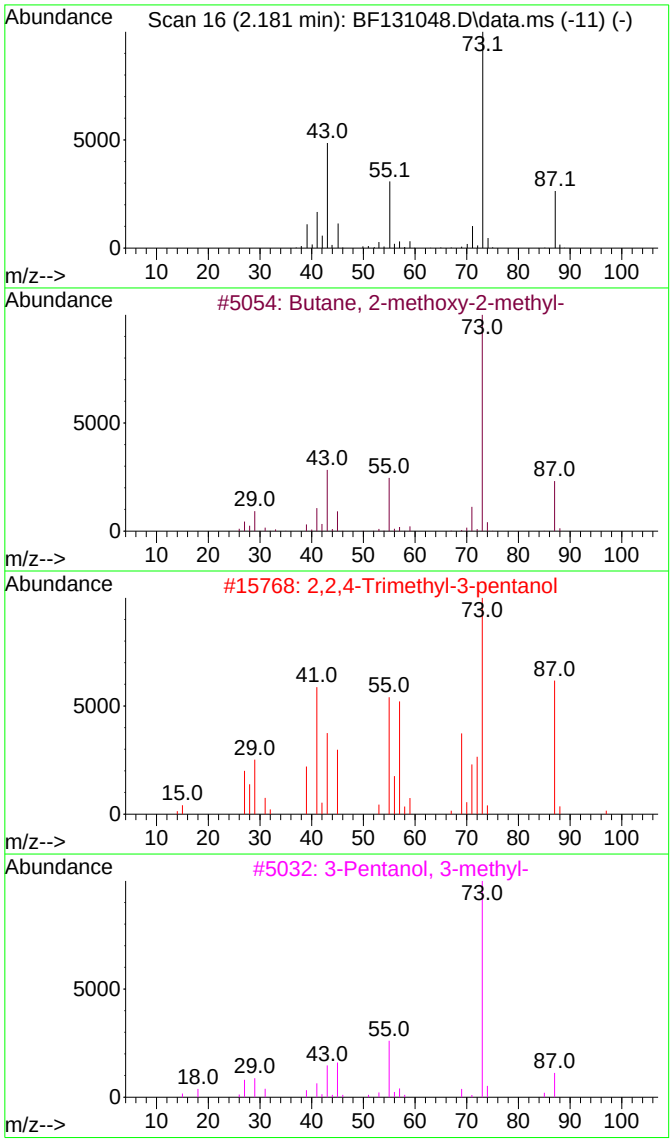
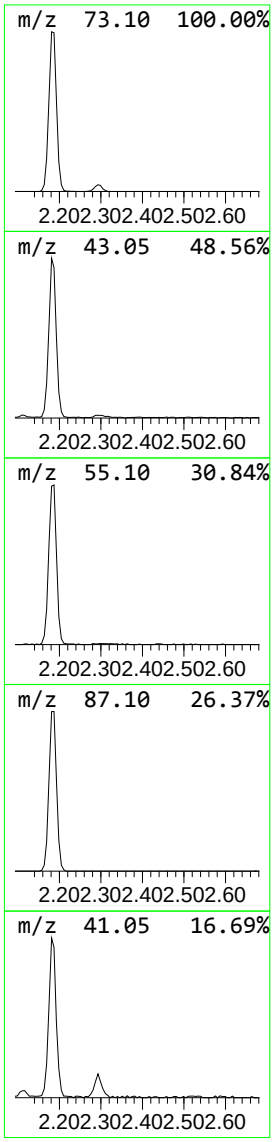
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	21.12 ng	594053	1,4-Dichlorobenzene-d4	6.898

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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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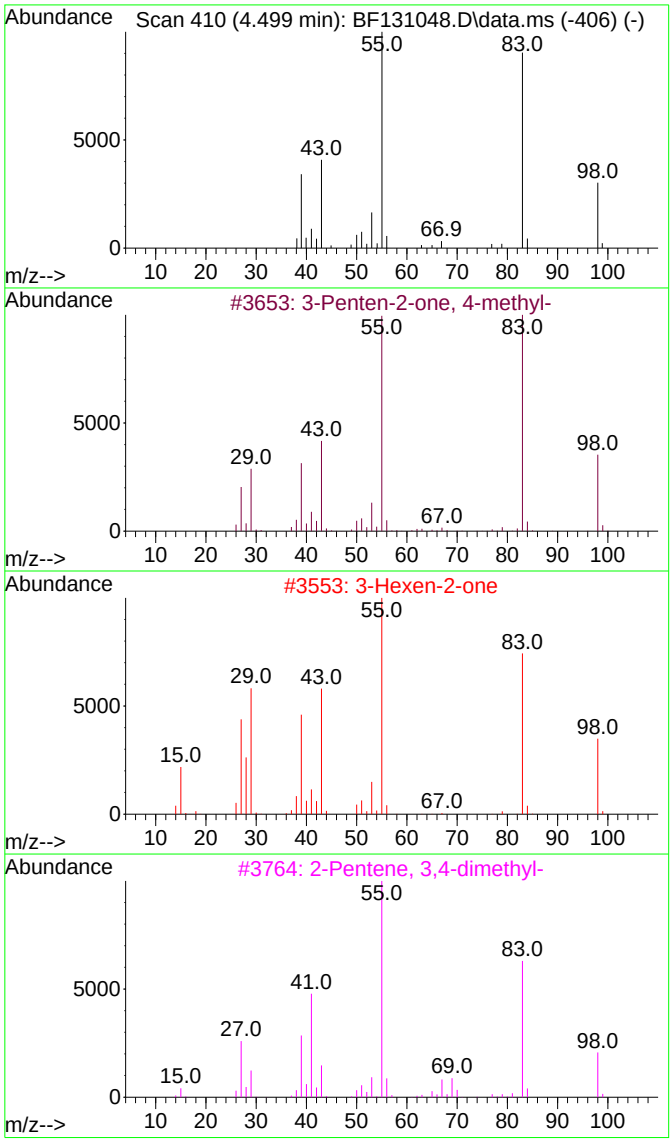
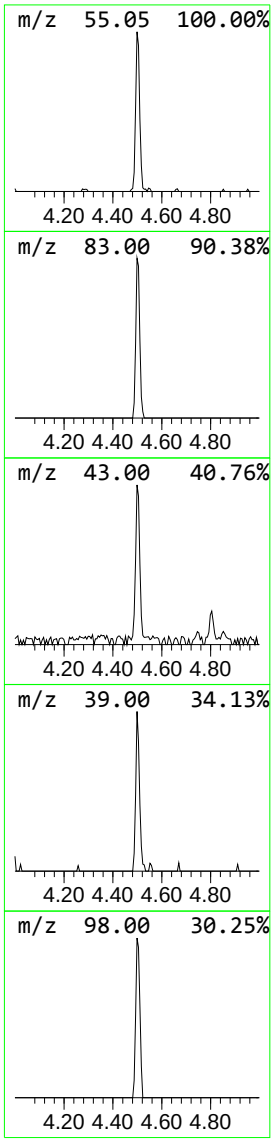
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.499	2.02 ng	56757	1,4-Dichlorobenzene-d4	6.898

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, 3,4-dimethyl-	98	C7H14	024910-63-2	72
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	72





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Sample : N5415-05
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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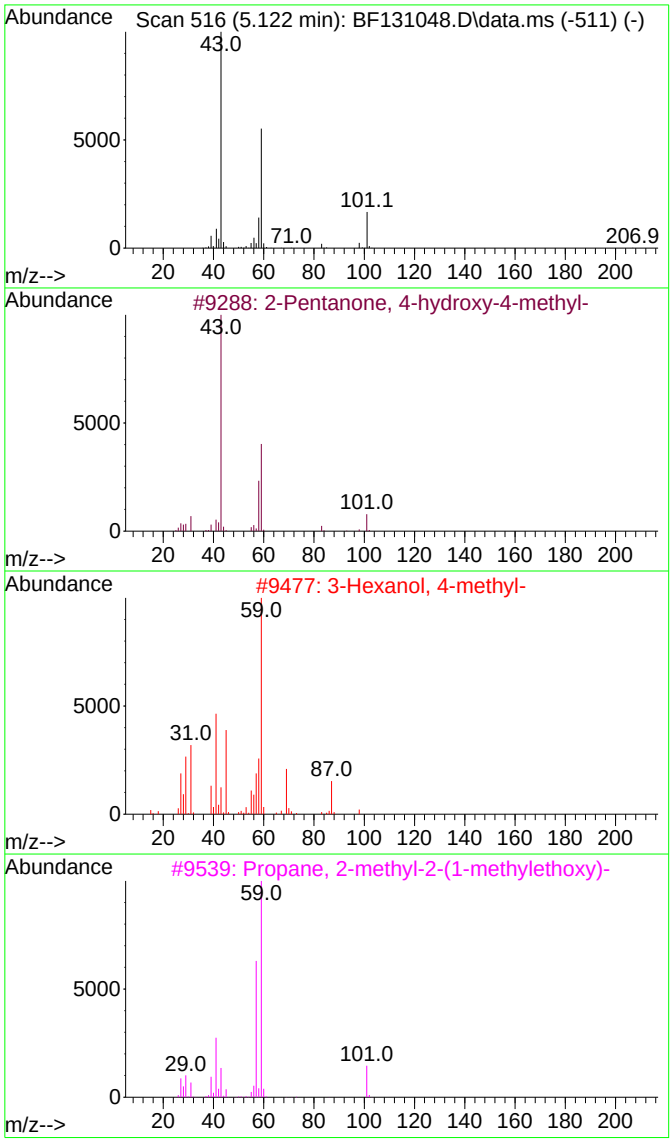
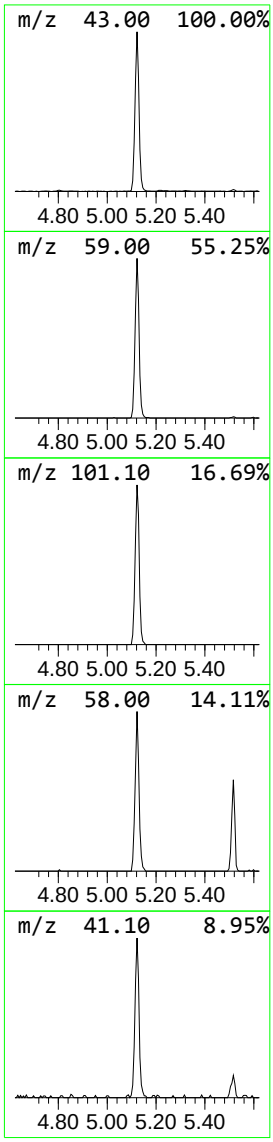
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	14.60 ng	410792	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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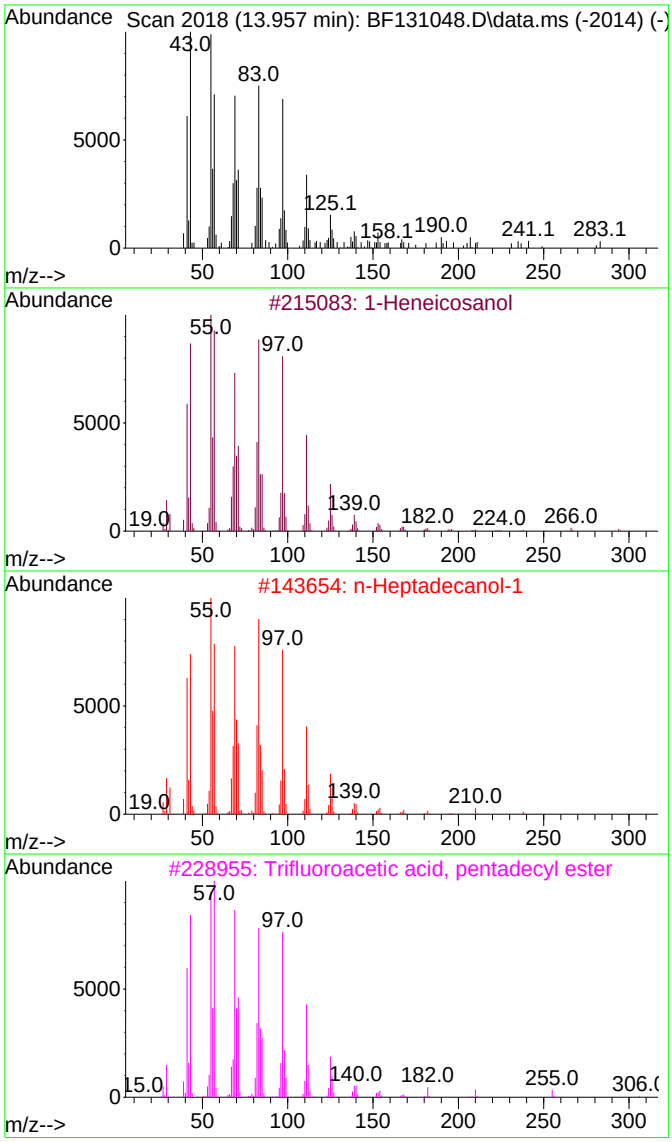
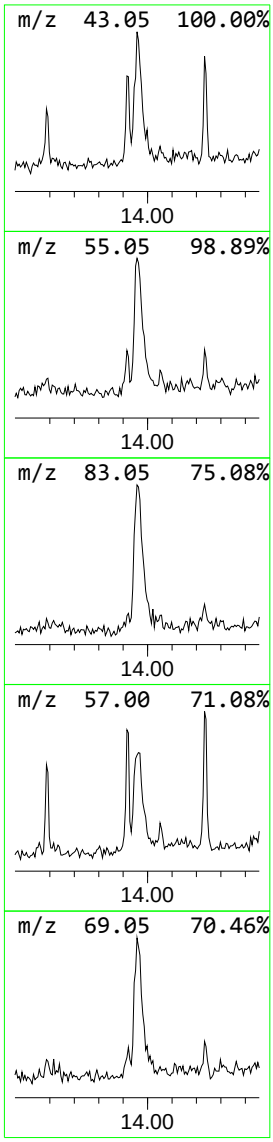
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	7.99 ng	184879	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93





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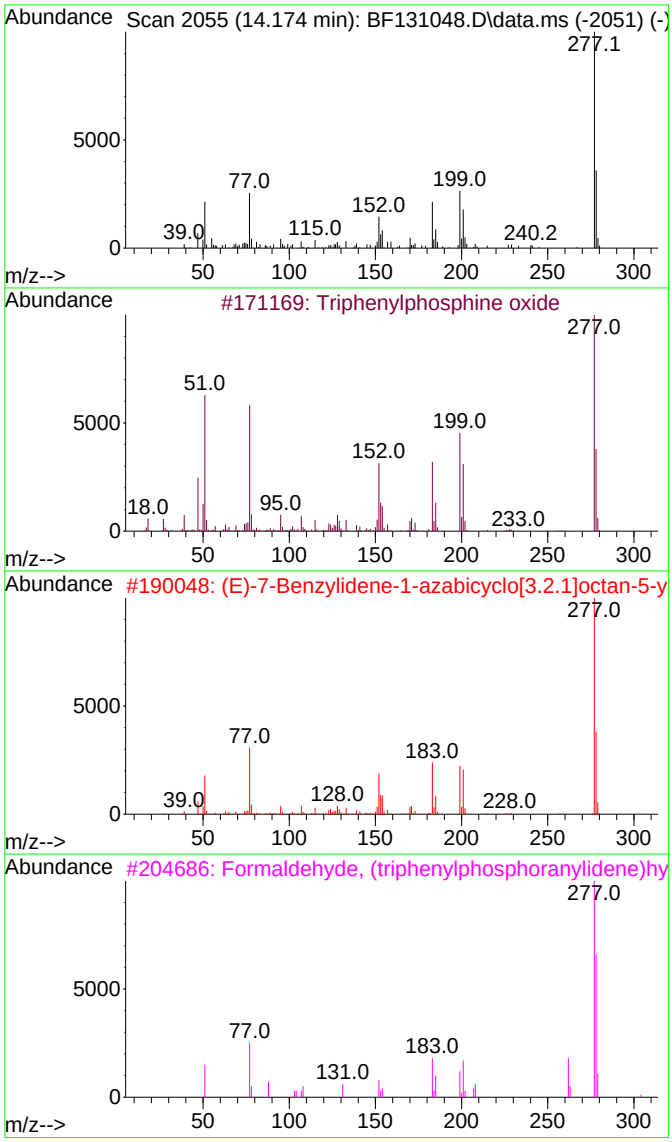
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

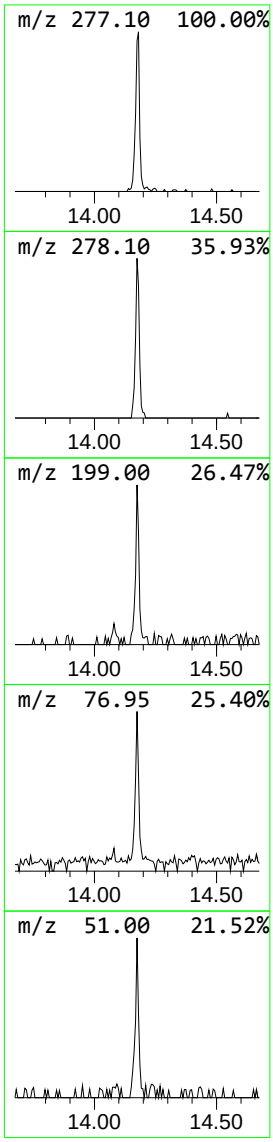
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	2.89 ng	66970	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
5	Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	40





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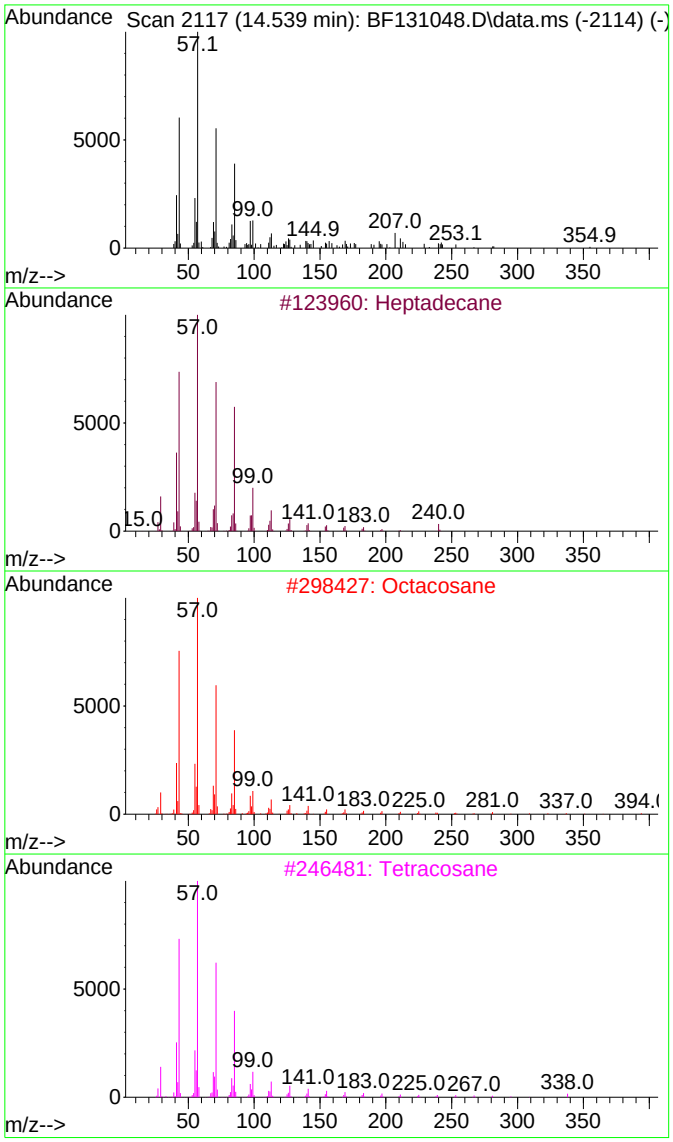
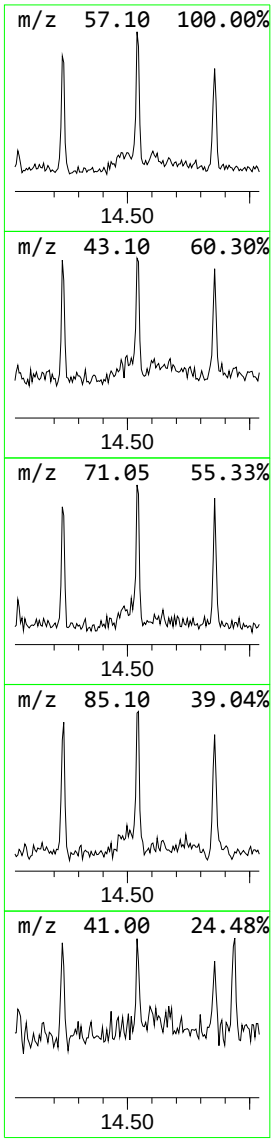
Peak Number 6 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.02 ng	46641	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Octacosane	394	C28H58	000630-02-4	80
3	Tetracosane	338	C24H50	000646-31-1	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	Eicosane	282	C20H42	000112-95-8	72





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.181	21.1	ng	594053	1	6.898	562621	20.0
3-Penten-2-one,...	4.499	2.0	ng	56757	1	6.898	562621	20.0
2-Pentanone, 4-...	5.122	14.6	ng	410792	1	6.898	562621	20.0
1-Heneicosanol	13.957	8.0	ng	184879	5	14.080	462863	20.0
Triphenylphosph...	14.174	2.9	ng	66970	5	14.080	462863	20.0
Heptadecane	14.539	2.0	ng	46641	5	14.080	462863	20.0