LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120222\
Data File : BF131495.D
Acq On : 02 Dec 2022 14:47
Operator : CG\JU
Sample : N5793-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-2022-11-28

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: BF131495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	28	rVB	1489804	1952920	62.29%	10.171%
2	4.528	409	415	420	rBV	49892	56303	1.80%	0.293%
3	5.151	514	521	524	rBV	877343	1059317	33.79%	5.517%
4	5.540	582	587	590	rBV	1450828	1281946	40.89%	6.677%
5	5.934	651	654	658	rBV	107713	95284	3.04%	0.496%
6	6.545	753	758	761	rBV	965532	876169	27.95%	4.563%
7	6.928	819	823	826	rVB	478670	396144	12.64%	2.063%
8	7.492	913	919	922	rBV	1411882	1416100	45.17%	7.375%
9	8.216	1037	1042	1045	rBV	808647	696902	22.23%	3.630%
10	9.298	1220	1226	1229	rBV	3391175	3102796	98.97%	16.160%
11	9.981	1337	1342	1345	rBV	993957	813632	25.95%	4.238%
12	10.775	1472	1477	1480	rBV	2064137	1903358	60.71%	9.913%
13	11.475	1592	1596	1600	rBV	978813	834012	26.60%	4.344%
14	11.539	1604	1607	1611	rVB3	40427	32953	1.05%	0.172%
15	13.074	1863	1868	1871	rBV	3323518	3135054	100.00%	16.328%
16	14.133	2044	2048	2051	rBV	692544	658236	21.00%	3.428%
17	14.227	2060	2064	2069	rVB	64275	67954	2.17%	0.354%
18	14.457	2094	2103	2112	rBV8	20381	59047	1.88%	0.308%
19	14.598	2121	2127	2130	rBV	29273	38652	1.23%	0.201%
20	14.633	2130	2133	2143	rVB7	18372	45175	1.44%	0.235%
21	15.657	2301	2307	2316	rBV	436298	571151	18.22%	2.975%
22	17.309	2577	2588	2601	rBV	27038	107196	3.42%	0.558%

Sum of corrected areas: 19200301

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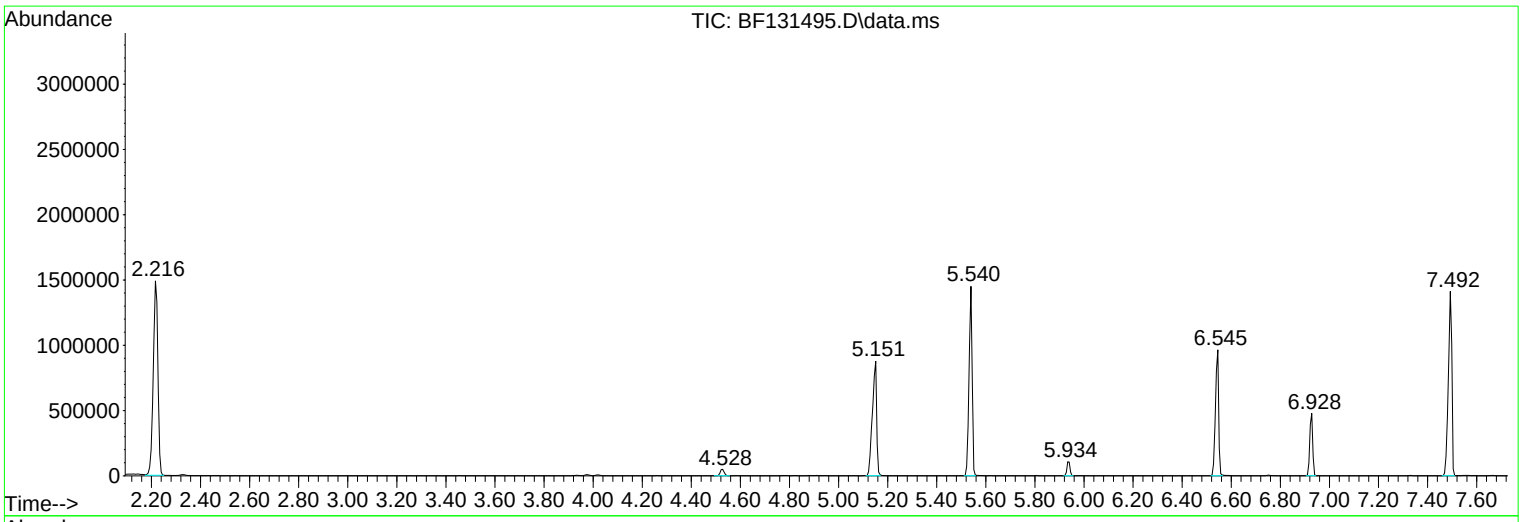
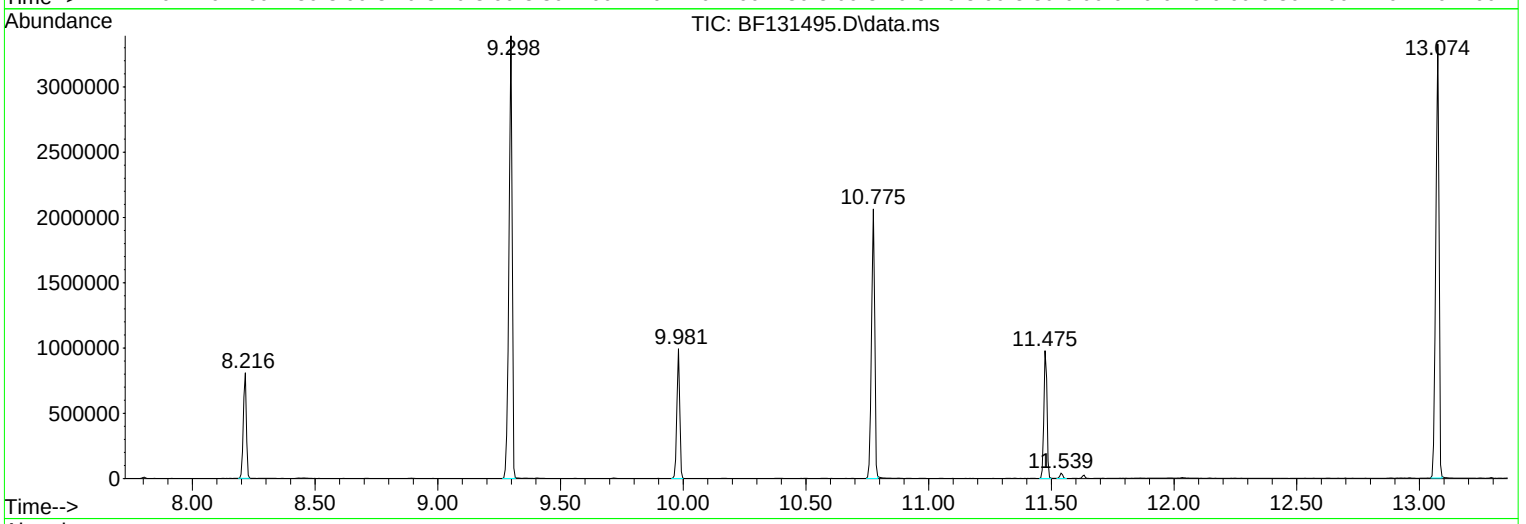
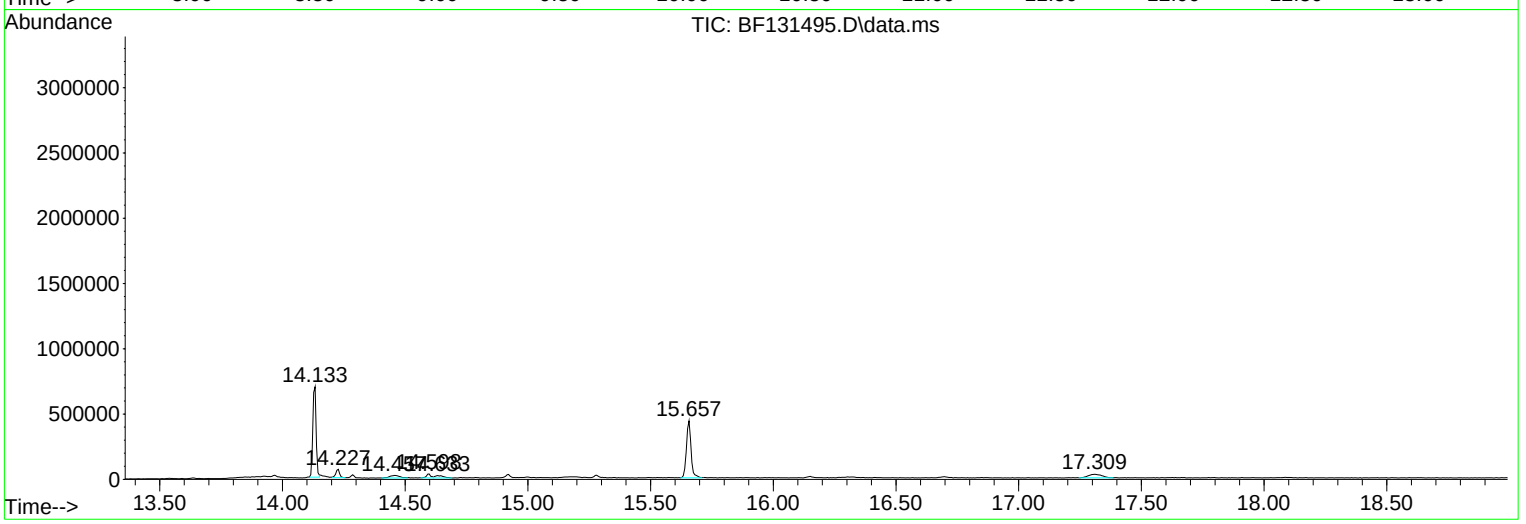
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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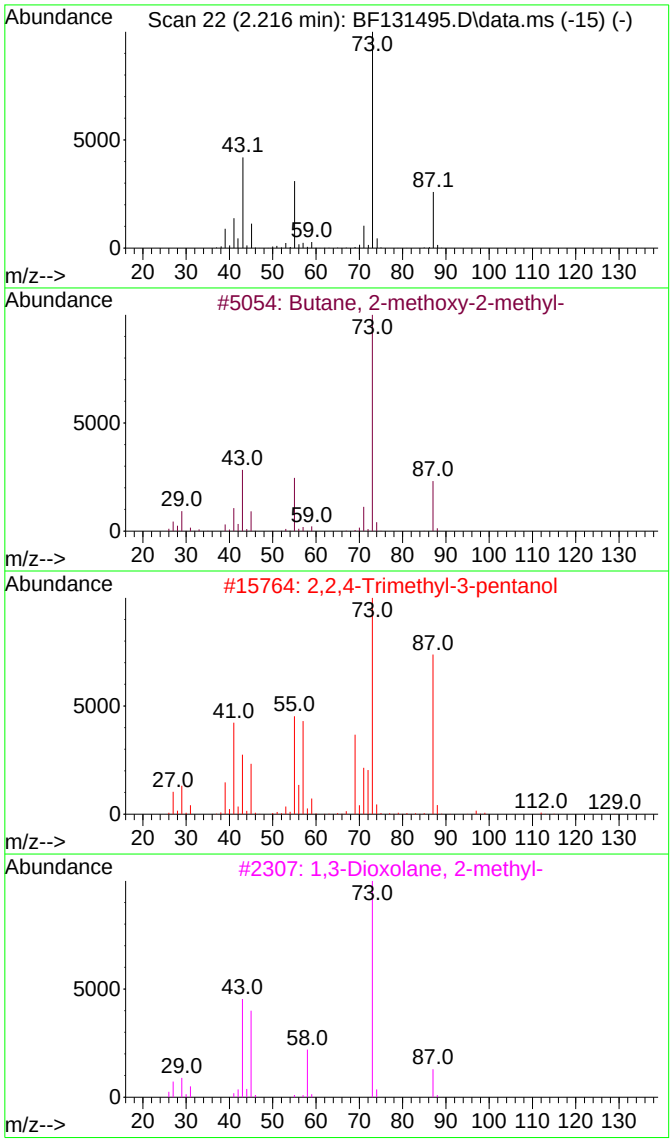
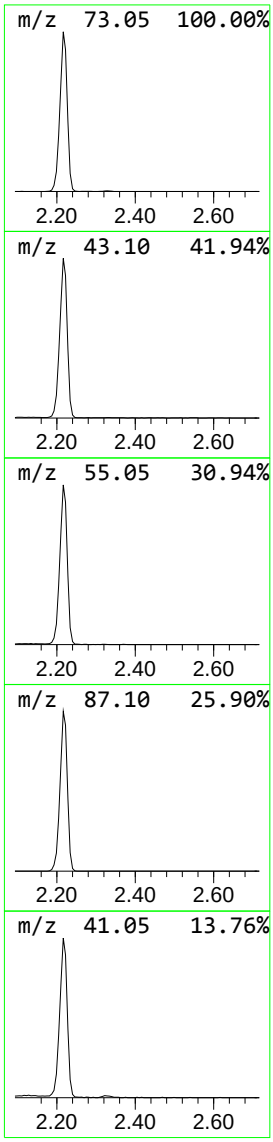
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	98.60 ng	1952920	1,4-Dichlorobenzene-d4	6.928

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	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
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TIC Library : C:\Database\NIST20.L
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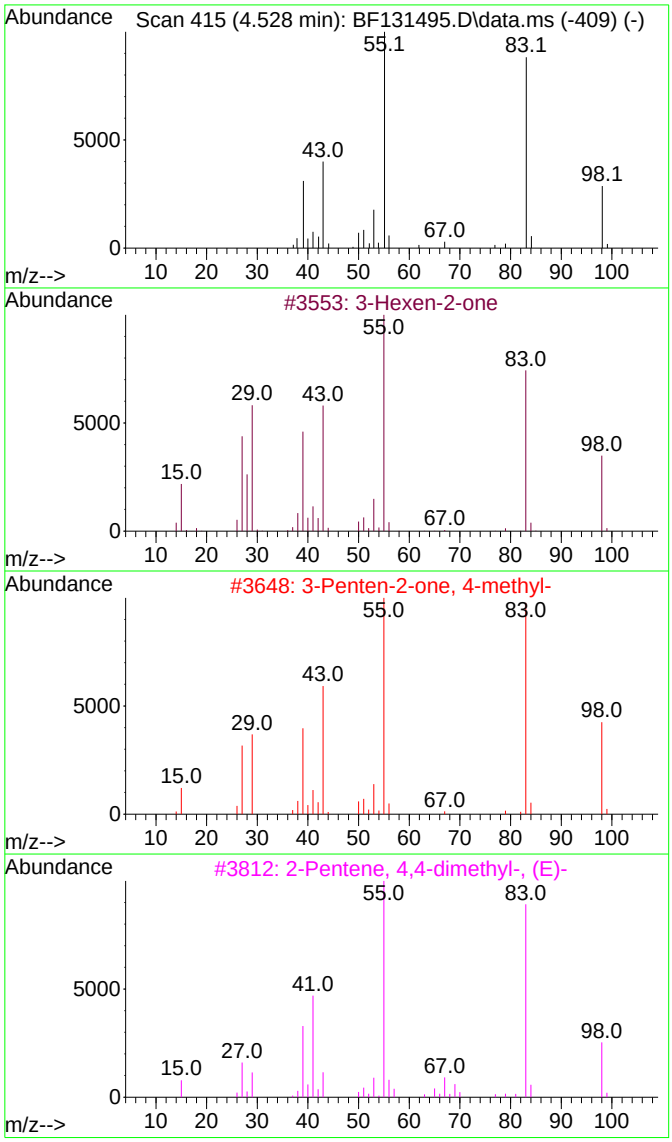
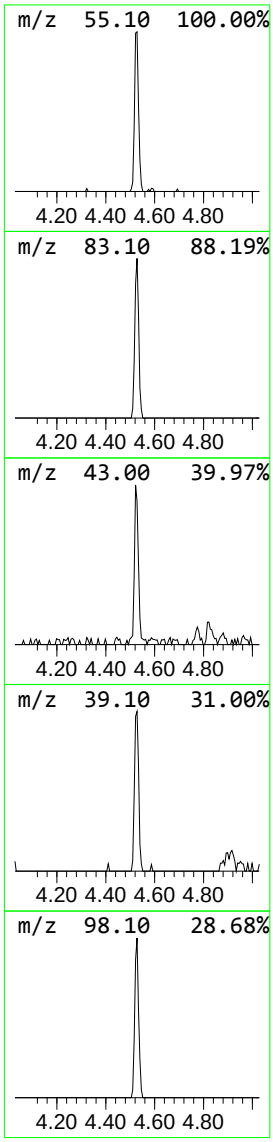
****

Peak Number 2 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.528	2.84 ng	56303	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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BNA_F
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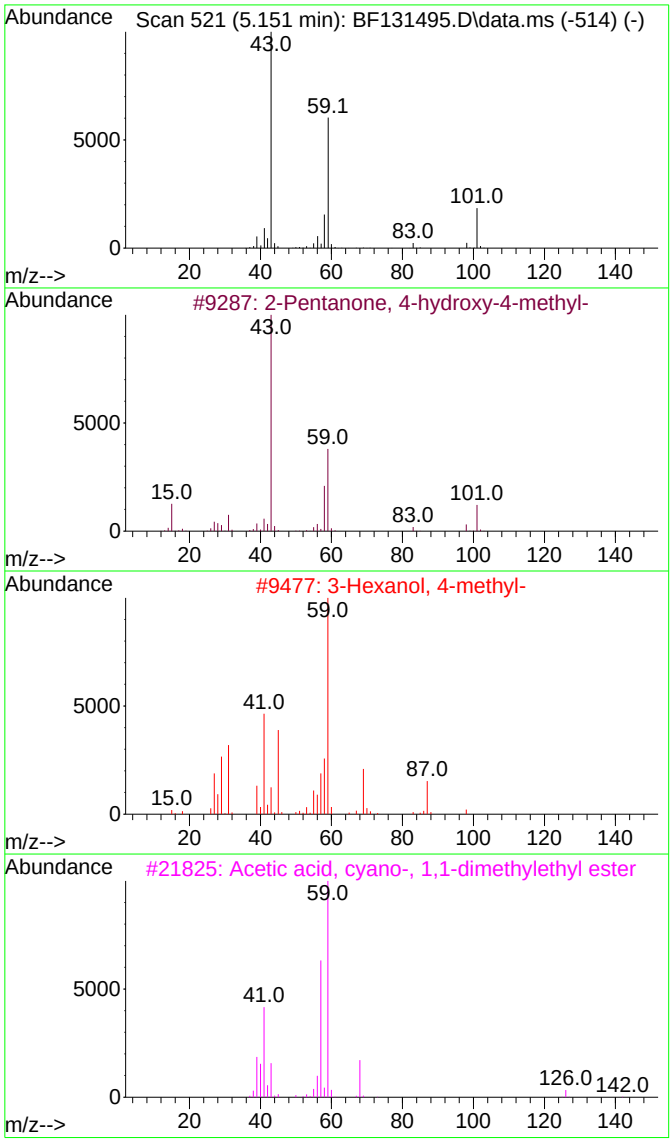
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

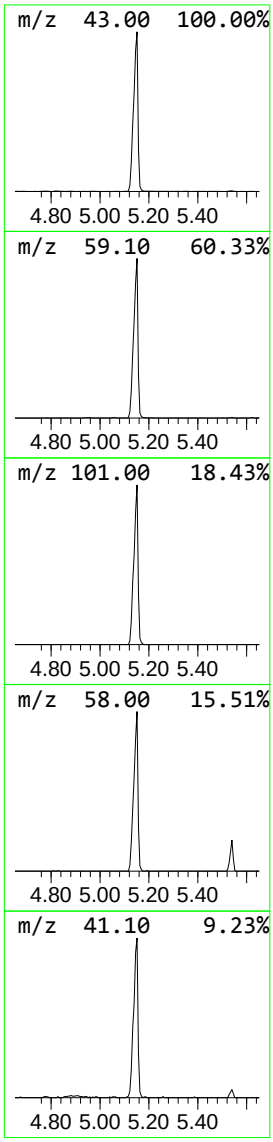
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	53.48 ng	1059320	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	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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Misc :
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Instrument :
BNA_F
ClientSampleId :
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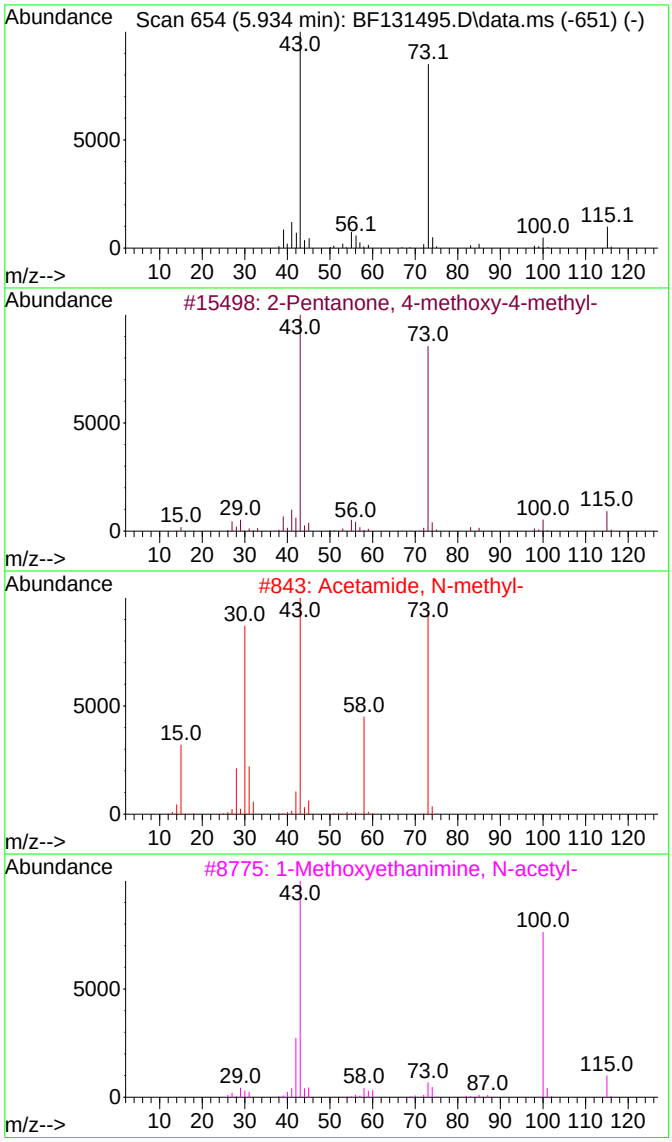
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

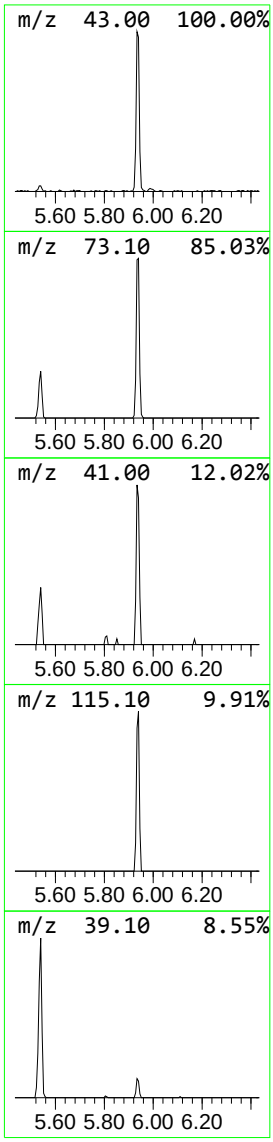
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.934	4.81 ng	95284	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	49
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	47
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
5	3-Hexanol, acetate	144	C8H16O2	040780-64-1	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
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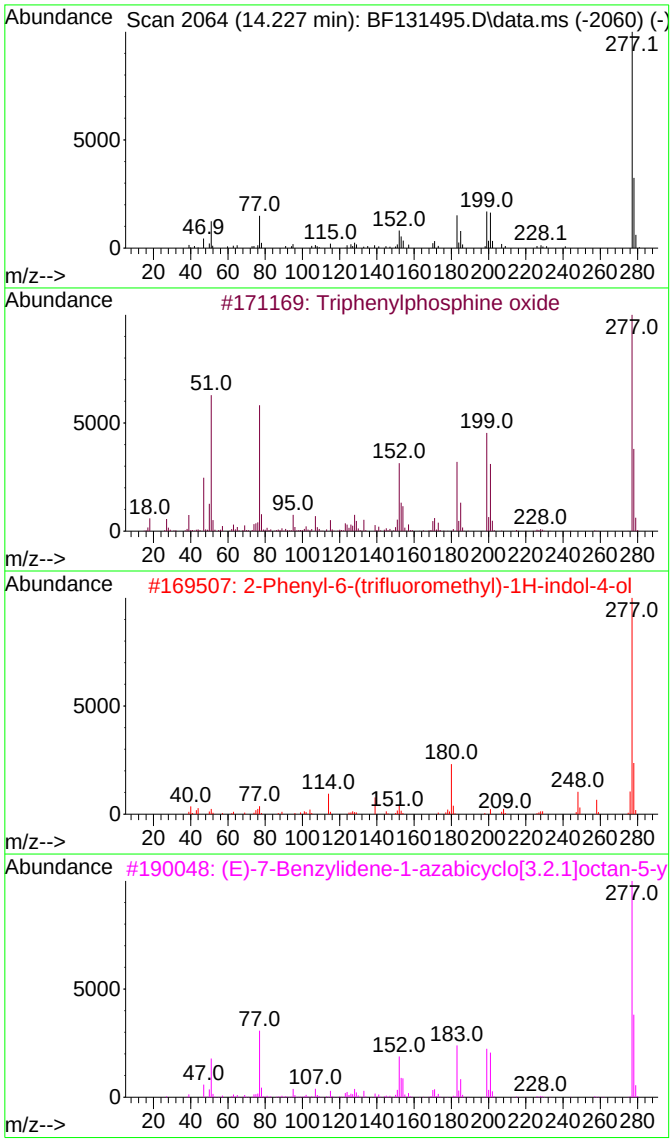
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

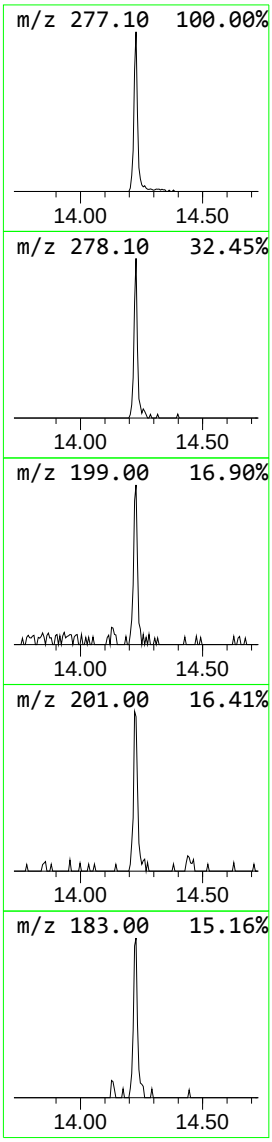
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	2.06 ng	67954	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	53
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	53
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	45
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38





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TIC Library : C:\Database\NIST20.L
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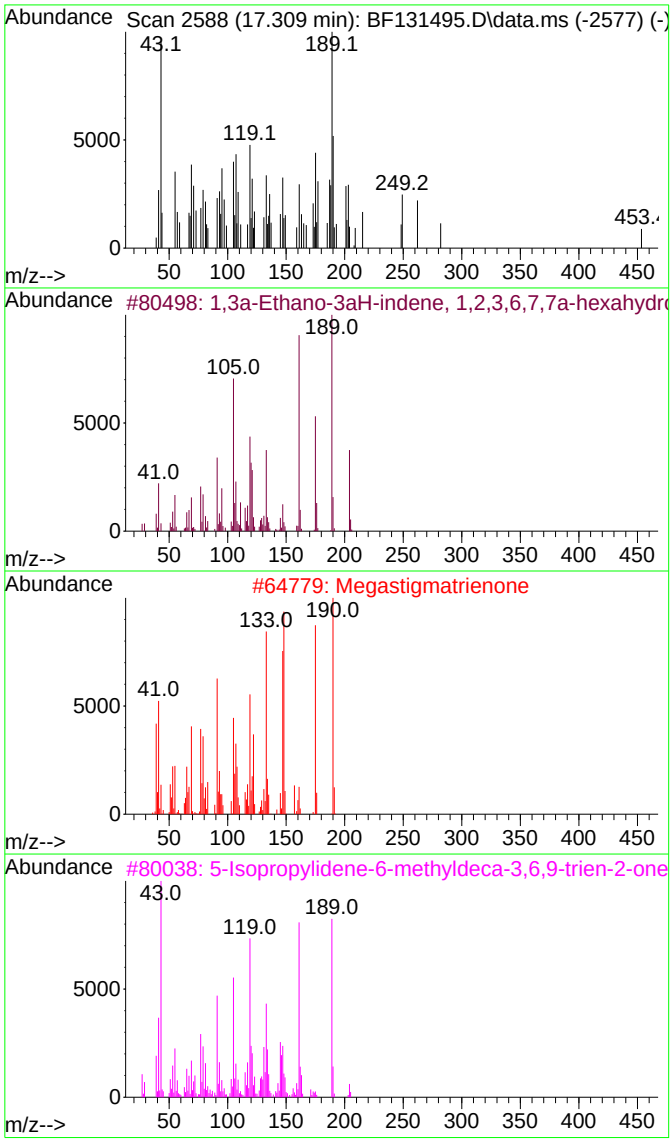
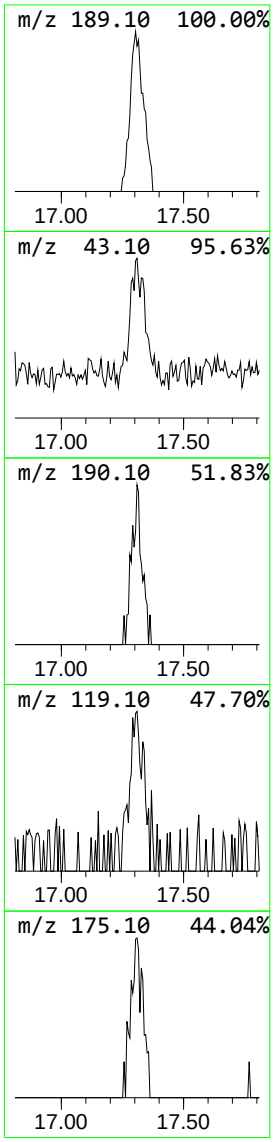
Peak Number 6 unknown17.310 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.310	3.75 ng	107196	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43
2	Megastigmatrienone	190	C13H18O	038818-55-2	38
3	5-Isopropylidene-6-methyldeca-3,...	204	C14H20O	1000197-84-7	38
4	6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	38
5	Methyl (S)-5-((1S,2R,4aR,8aR)-5-...	350	C22H38O3	1010495-83-9	38





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.216	98.6	ng	1952920	1	6.928	396144	20.0
3-Hexen-2-one	4.528	2.8	ng	56303	1	6.928	396144	20.0
2-Pentanone, 4-...	5.151	53.5	ng	1059320	1	6.928	396144	20.0
2-Pentanone, 4-...	5.934	4.8	ng	95284	1	6.928	396144	20.0
Triphenylphosph...	14.227	2.1	ng	67954	5	14.133	658236	20.0
unknown17.310	17.310	3.8	ng	107196	6	15.657	571151	20.0