LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131104.D
Acq On : 10 Nov 2022 00:06
Operator : CG\JU
Sample : N5360-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221171-COMP-06-MODIFIED-ELUTRIATE

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: BF131104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	20	rVB	1076633	1303212	67.49%	10.807%
2	2.275	28	32	37	rVB	30453	36434	1.89%	0.302%
3	5.104	509	513	519	rBV	155272	151796	7.86%	1.259%
4	5.504	577	581	593	rBV	804121	685929	35.52%	5.688%
5	6.510	749	752	761	rBV	643134	554606	28.72%	4.599%
6	6.887	813	816	820	rBV	571342	525779	27.23%	4.360%
7	7.457	905	913	916	rBV	1241464	1226119	63.50%	10.168%
8	8.175	1031	1035	1038	rBV	838344	676823	35.05%	5.613%
9	9.251	1213	1218	1221	rBV	2370815	1931007	100.00%	16.014%
10	9.645	1281	1285	1288	rBV	41465	30922	1.60%	0.256%
11	9.934	1325	1334	1337	rBV	915379	781518	40.47%	6.481%
12	10.269	1388	1391	1394	rBV	39827	30586	1.58%	0.254%
13	10.722	1464	1468	1472	rBV	1312091	1179673	61.09%	9.783%
14	11.422	1583	1587	1591	rBV	900415	793138	41.07%	6.577%
15	13.010	1853	1857	1860	rBV	984008	793555	41.10%	6.581%
16	13.927	2004	2013	2026	rBV	99905	215766	11.17%	1.789%
17	14.069	2034	2037	2041	rBV	644356	541587	28.05%	4.491%
18	14.163	2048	2053	2059	rBV	86128	92744	4.80%	0.769%
19	14.916	2178	2181	2186	rVB	48352	49694	2.57%	0.412%
20	15.563	2286	2291	2298	rBV	377194	457547	23.69%	3.794%

Sum of corrected areas: 12058435

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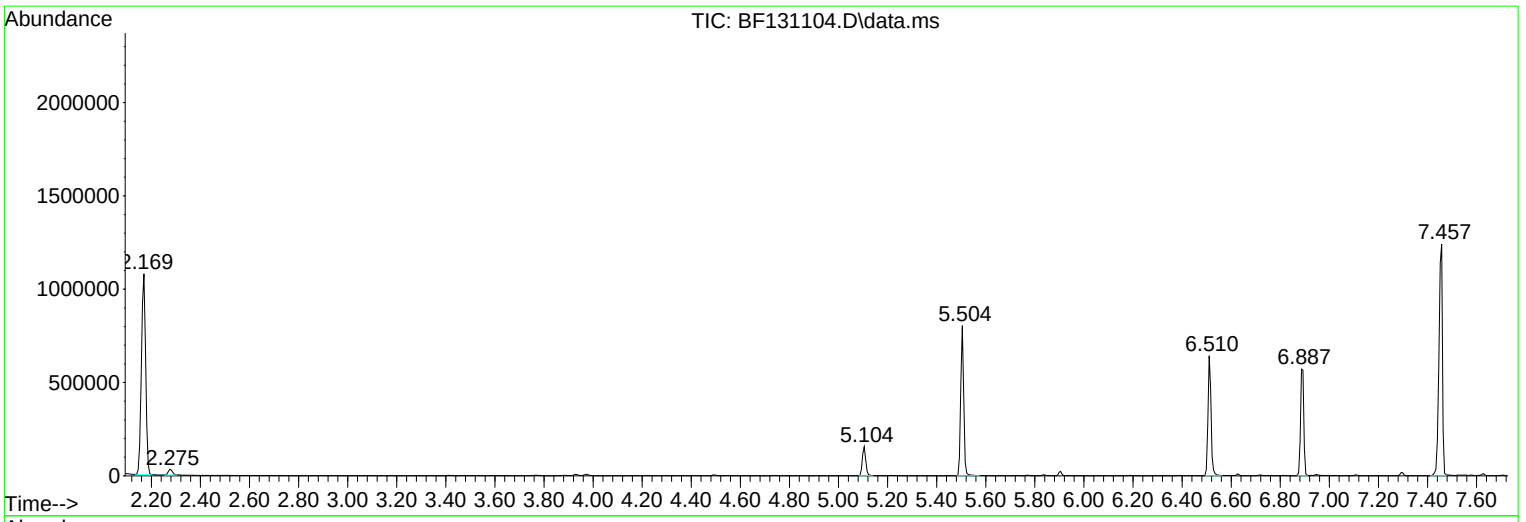
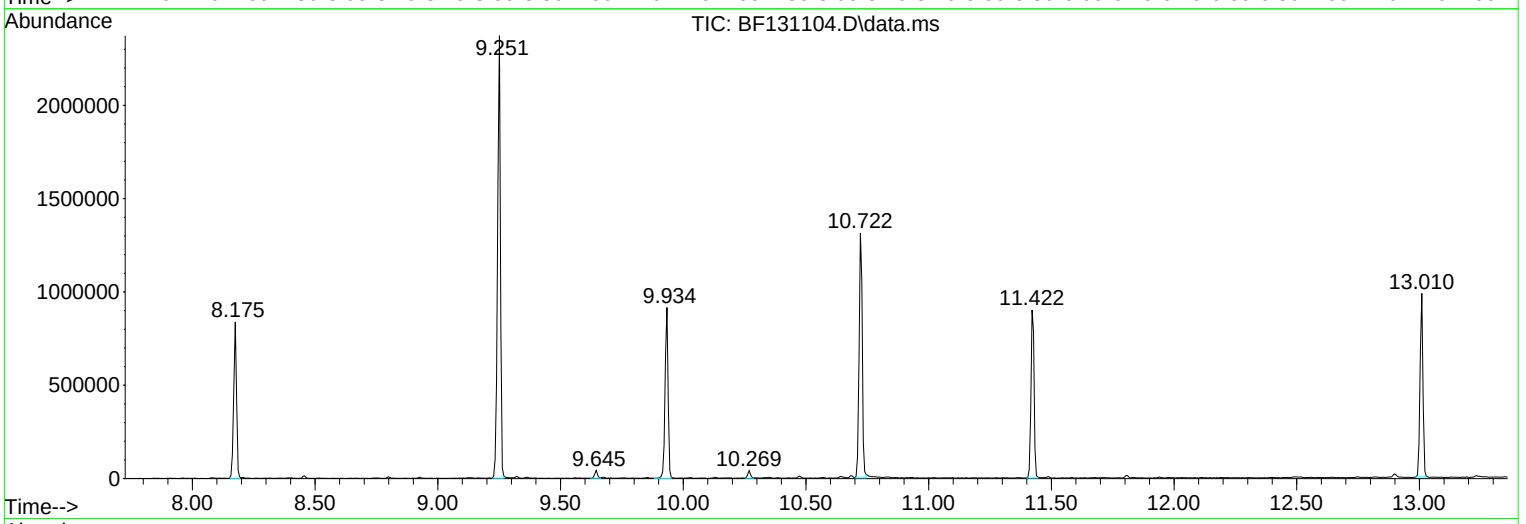
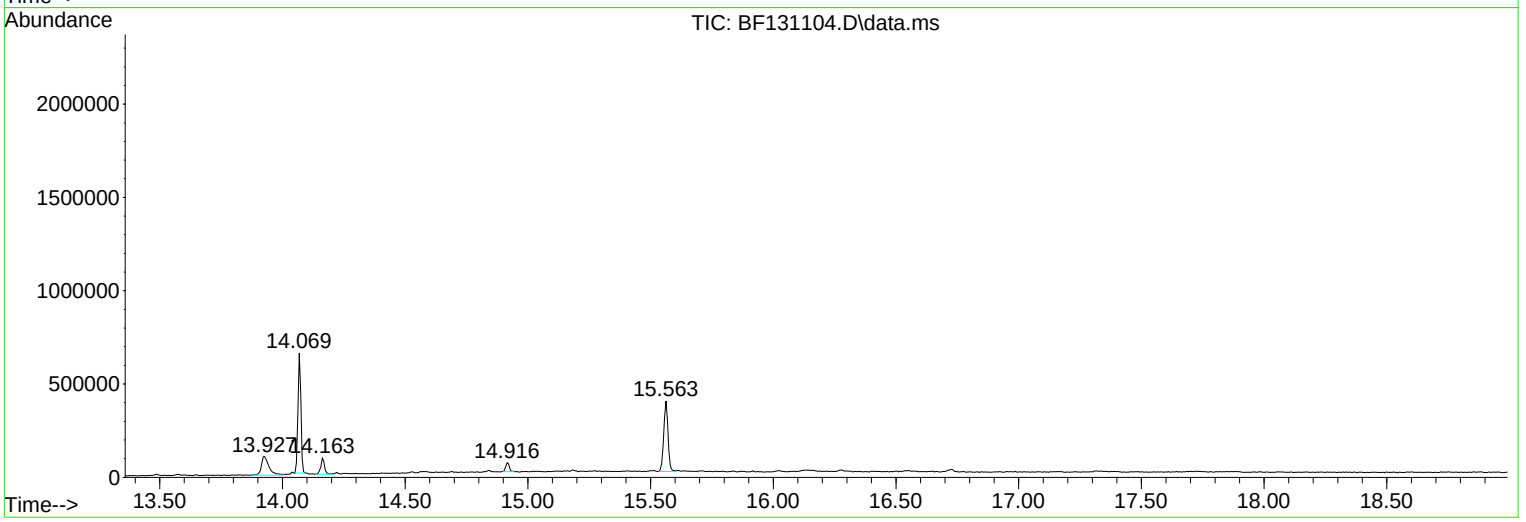
ClientSampleId :
DISSOLVED-20221171-COMP-06-MODIFIED-ELUTRIATE

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

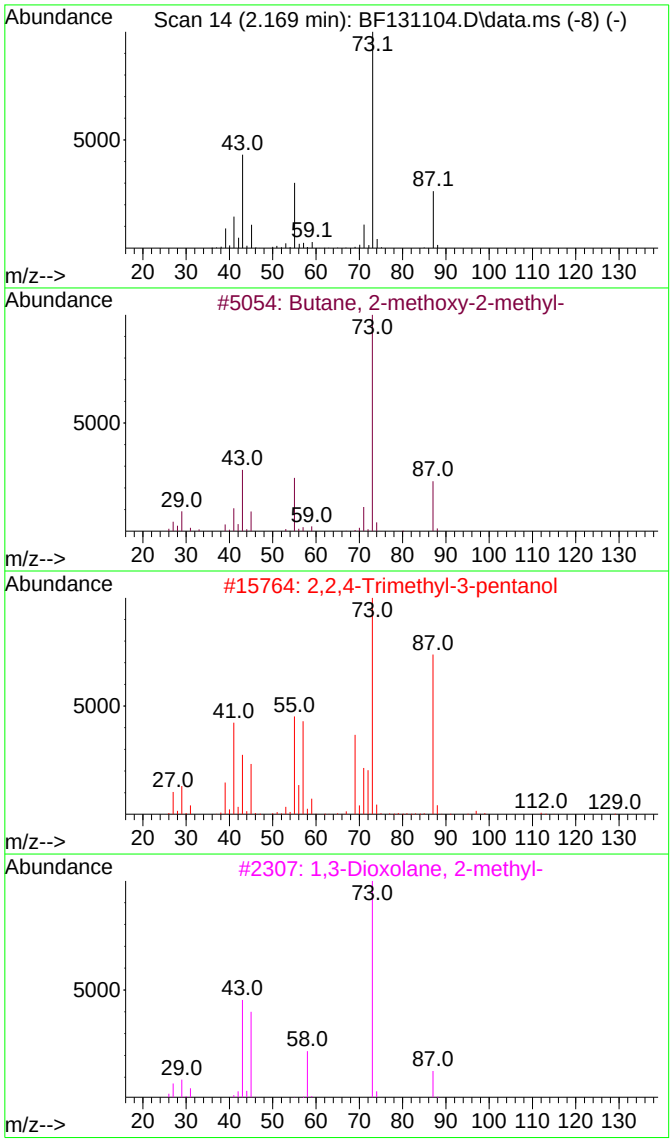
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

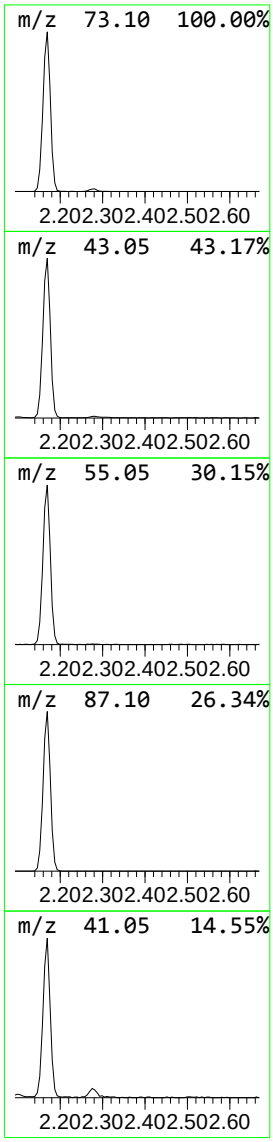
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	49.57 ng	1303210	1,4-Dichlorobenzene-d4	6.893

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	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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BNA_F
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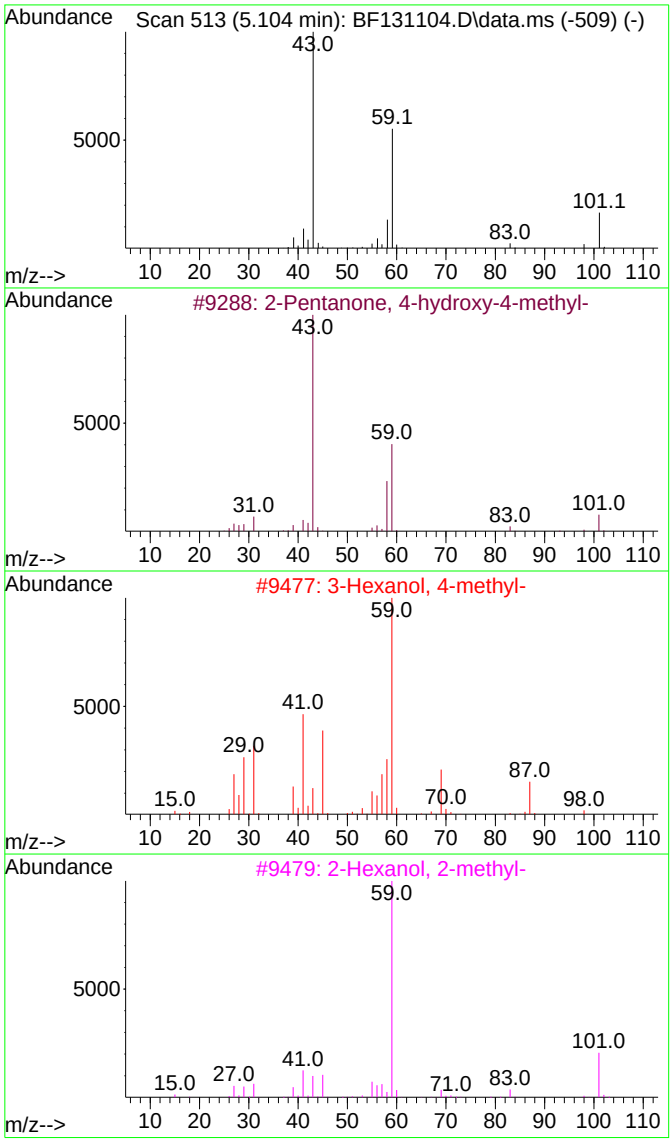
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

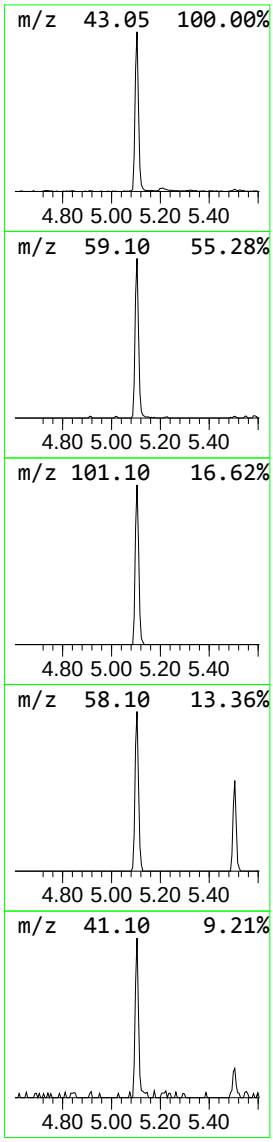
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.77 ng	151796	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131104.D
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Operator : CG\JU
Sample : N5360-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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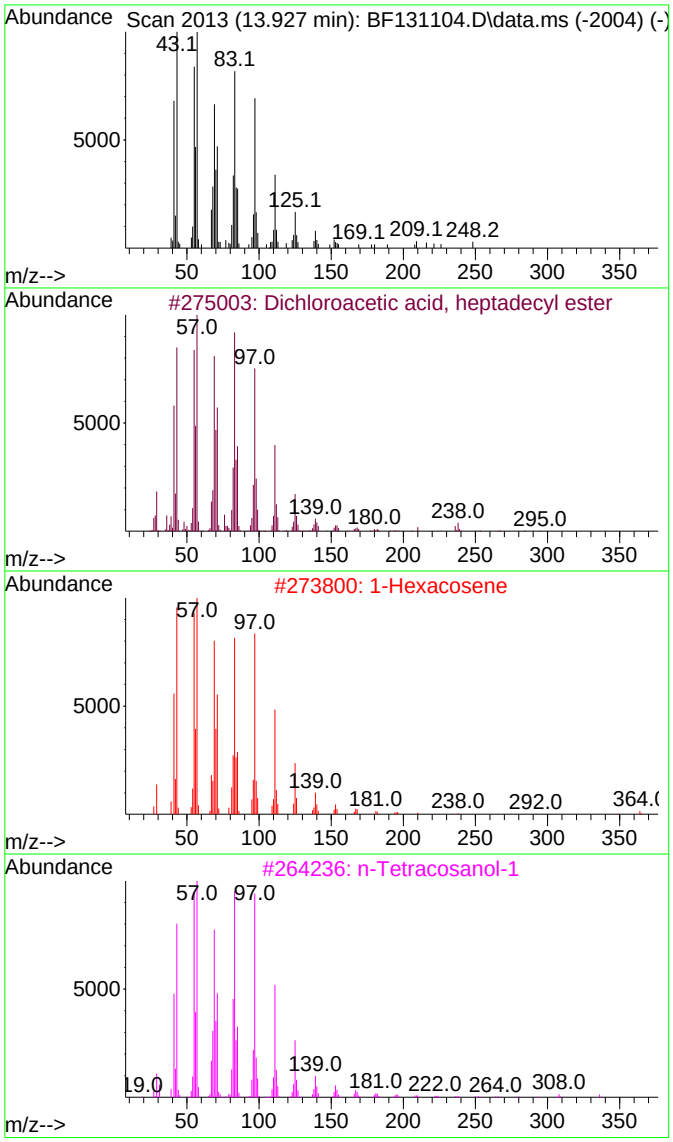
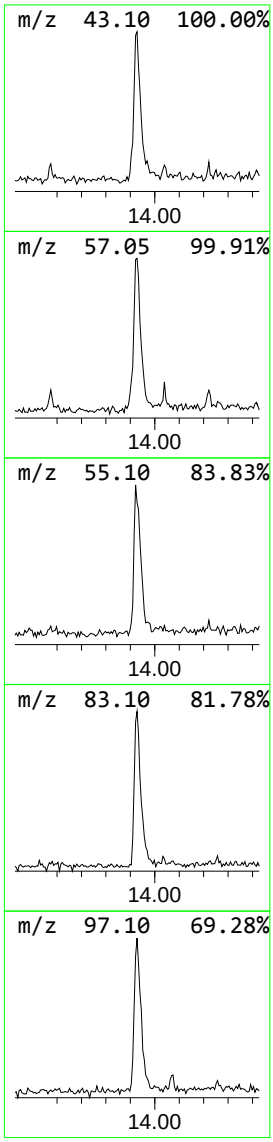
****
Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	7.97 ng	215766	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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TIC Library : C:\Database\NIST20.L
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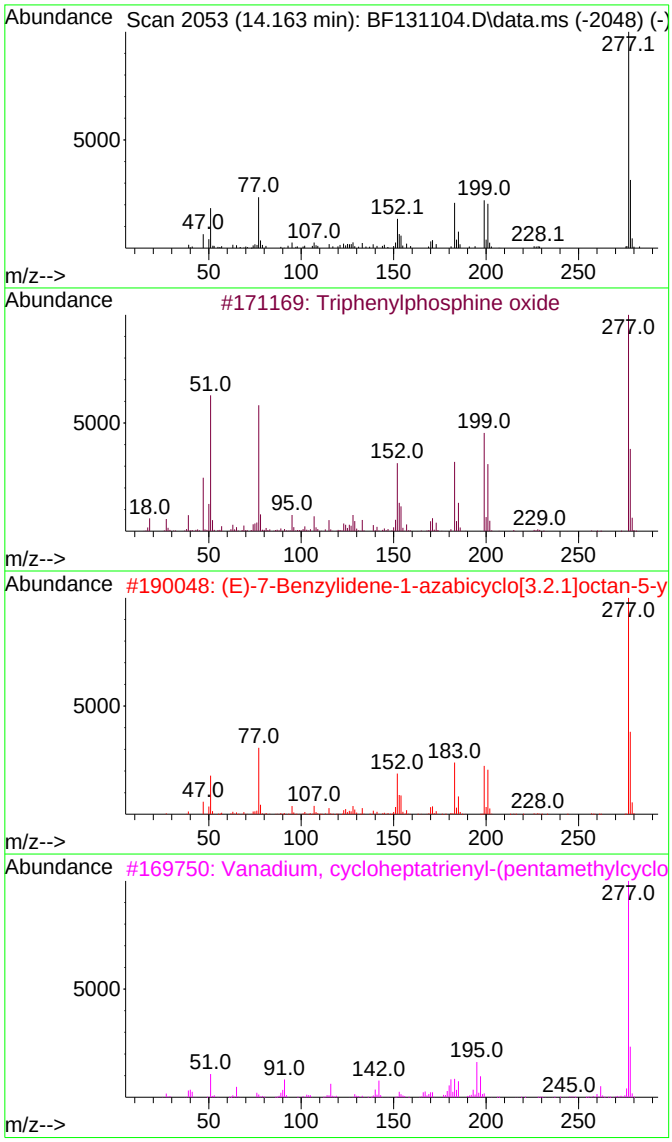
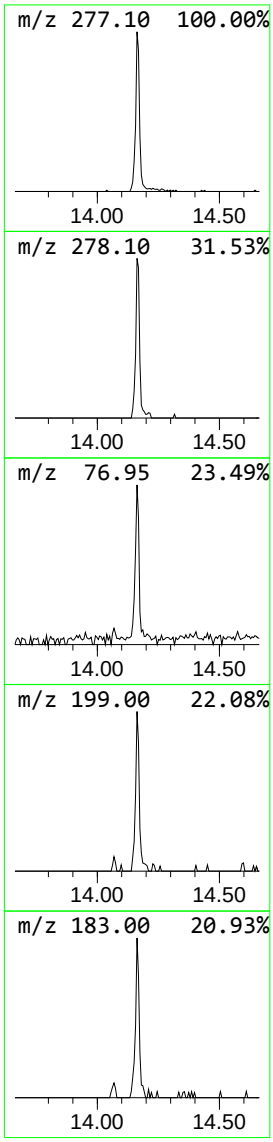
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	3.42 ng	92744	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	76
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	36





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ALS Vial : 13 Sample Multiplier: 1

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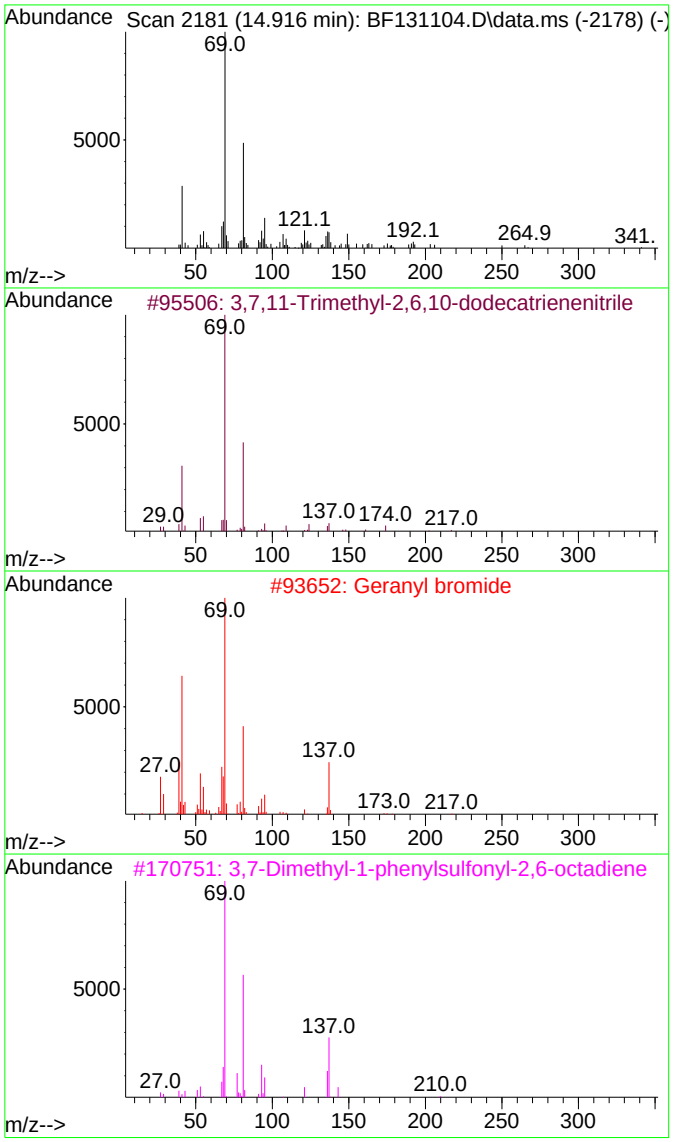
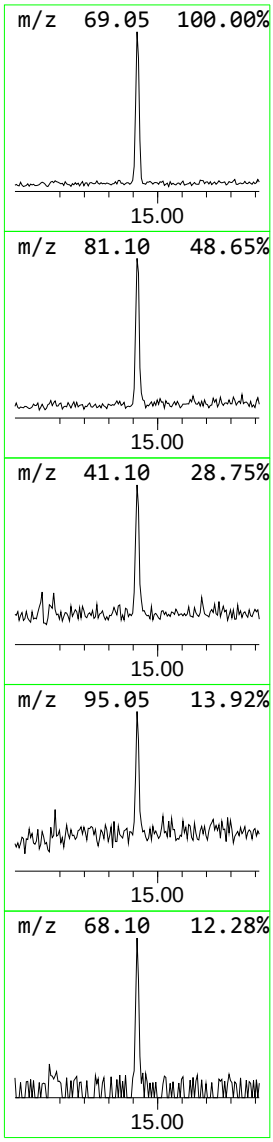
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3,7,11-Trimethyl-2,6,10-dod... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	2.17 ng	49694	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
2	Geranyl bromide	216	C10H17Br	006138-90-5	64
3	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59





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...	2.169	49.6	ng	1303210	1	6.893	525779	20.0
2-Pentanone, 4-...	5.104	5.8	ng	151796	1	6.893	525779	20.0
Dichloroacetic ...	13.927	8.0	ng	215766	5	14.069	541587	20.0
Triphenylphosph...	14.163	3.4	ng	92744	5	14.069	541587	20.0
3,7,11-Trimethy...	14.916	2.2	ng	49694	6	15.563	457547	20.0