LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125332.D
Acq On : 2 Sep 2021 21:16
Operator : JU/CG
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-1

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	7	12	18	rVB	649285	818479	40.31%	3.692%
2	5.522	580	584	595	rBV	2105740	1871204	92.16%	8.442%
3	6.151	685	691	694	rBV2	17751	26617	1.31%	0.120%
4	6.440	736	740	746	rBV4	21711	26092	1.29%	0.118%
5	6.534	751	756	763	rBV	1860679	1891669	93.17%	8.534%
6	6.904	816	819	823	rVB	1287887	1035077	50.98%	4.670%
7	7.057	841	845	848	rBV4	26729	32849	1.62%	0.148%
8	7.175	859	865	869	rVB4	20072	27046	1.33%	0.122%
9	7.440	903	910	911	rBV4	16129	25161	1.24%	0.114%
10	7.469	911	915	924	rVV	1318344	1203955	59.30%	5.431%
11	7.545	924	928	931	rVB4	20867	31396	1.55%	0.142%
12	8.063	1012	1016	1018	rBV2	23088	25327	1.25%	0.114%
13	8.092	1018	1021	1025	rBV2	45010	75656	3.73%	0.341%
14	8.192	1034	1038	1044	rBV	1490765	1342876	66.14%	6.058%
15	8.245	1044	1047	1049	rVB	78675	68307	3.36%	0.308%
16	8.392	1069	1072	1075	rVB3	50365	38844	1.91%	0.175%
17	8.475	1080	1086	1093	rBV7	36427	57640	2.84%	0.260%
18	8.534	1093	1096	1099	rBV3	19702	26532	1.31%	0.120%
19	8.604	1105	1108	1110	rBV	115884	90176	4.44%	0.407%
20	8.728	1125	1129	1131	rBV2	51679	45718	2.25%	0.206%
21	8.869	1150	1153	1156	rVB4	38710	48907	2.41%	0.221%
22	8.963	1167	1169	1172	rBV3	24985	26026	1.28%	0.117%
23	9.069	1183	1187	1189	rBV4	26198	37938	1.87%	0.171%
24	9.092	1189	1191	1195	rVB3	23072	29227	1.44%	0.132%
25	9.204	1208	1210	1215	rVB2	114998	98941	4.87%	0.446%
26	9.263	1216	1220	1229	rBV	2460981	2030373	100.00%	9.160%
27	9.345	1230	1234	1236	rBV2	65476	72677	3.58%	0.328%
28	9.539	1263	1267	1268	rBV4	19209	26950	1.33%	0.122%
29	9.604	1275	1278	1281	rBV	577029	477892	23.54%	2.156%
30	9.657	1284	1287	1290	rVB2	297913	263469	12.98%	1.189%
31	9.810	1307	1313	1319	rBV	128775	159370	7.85%	0.719%
32	9.857	1319	1321	1323	rVB2	40789	31579	1.56%	0.142%
33	9.945	1333	1336	1340	rBV	1819225	1514723	74.60%	6.833%
34	10.145	1365	1370	1373	rVB7	20701	29253	1.44%	0.132%
35	10.357	1401	1406	1411	rBV8	22382	37435	1.84%	0.169%
36	10.586	1442	1445	1449	rBV3	43479	40708	2.00%	0.184%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125332.D
Acq On : 2 Sep 2021 21:16
Operator : JU/CG
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-1

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.675	1458	1460	1463	rBV2	38403	29511	1.45%	0.133%
38	10.733	1467	1470	1475	rVV	1476086	1326882	65.35%	5.986%
39	10.775	1475	1477	1480	rVB3	52436	47153	2.32%	0.213%
40	10.857	1485	1491	1497	rVB	57456	71678	3.53%	0.323%
41	10.910	1497	1500	1503	rBV	94647	74318	3.66%	0.335%
42	11.063	1519	1526	1529	rBV7	16008	34713	1.71%	0.157%
43	11.316	1566	1569	1576	rVB4	18302	26700	1.32%	0.120%
44	11.433	1585	1589	1596	rBV	1666588	1531993	75.45%	6.911%
45	11.716	1634	1637	1647	rVB10	12113	25064	1.23%	0.113%
46	11.951	1673	1677	1682	rBV3	57477	71439	3.52%	0.322%
47	12.527	1770	1775	1779	rBV2	135579	157637	7.76%	0.711%
48	12.651	1794	1796	1799	rBV	36680	28033	1.38%	0.126%
49	12.880	1830	1835	1839	rBV	47841	54607	2.69%	0.246%
50	13.016	1855	1858	1862	rBV	1643972	1490834	73.43%	6.726%
51	13.345	1910	1914	1918	rBV3	56942	76231	3.75%	0.344%
52	13.451	1927	1932	1935	rBV	804640	771537	38.00%	3.481%
53	13.486	1935	1938	1953	rVB4	169895	384220	18.92%	1.733%
54	13.886	2003	2006	2009	rBV2	68347	75320	3.71%	0.340%
55	14.080	2035	2039	2049	rVB	1090115	1067353	52.57%	4.815%
56	14.474	2104	2106	2110	rBV5	31724	37002	1.82%	0.167%
57	15.580	2289	2294	2302	rVB	809742	1098005	54.08%	4.953%

Sum of corrected areas: 22166319

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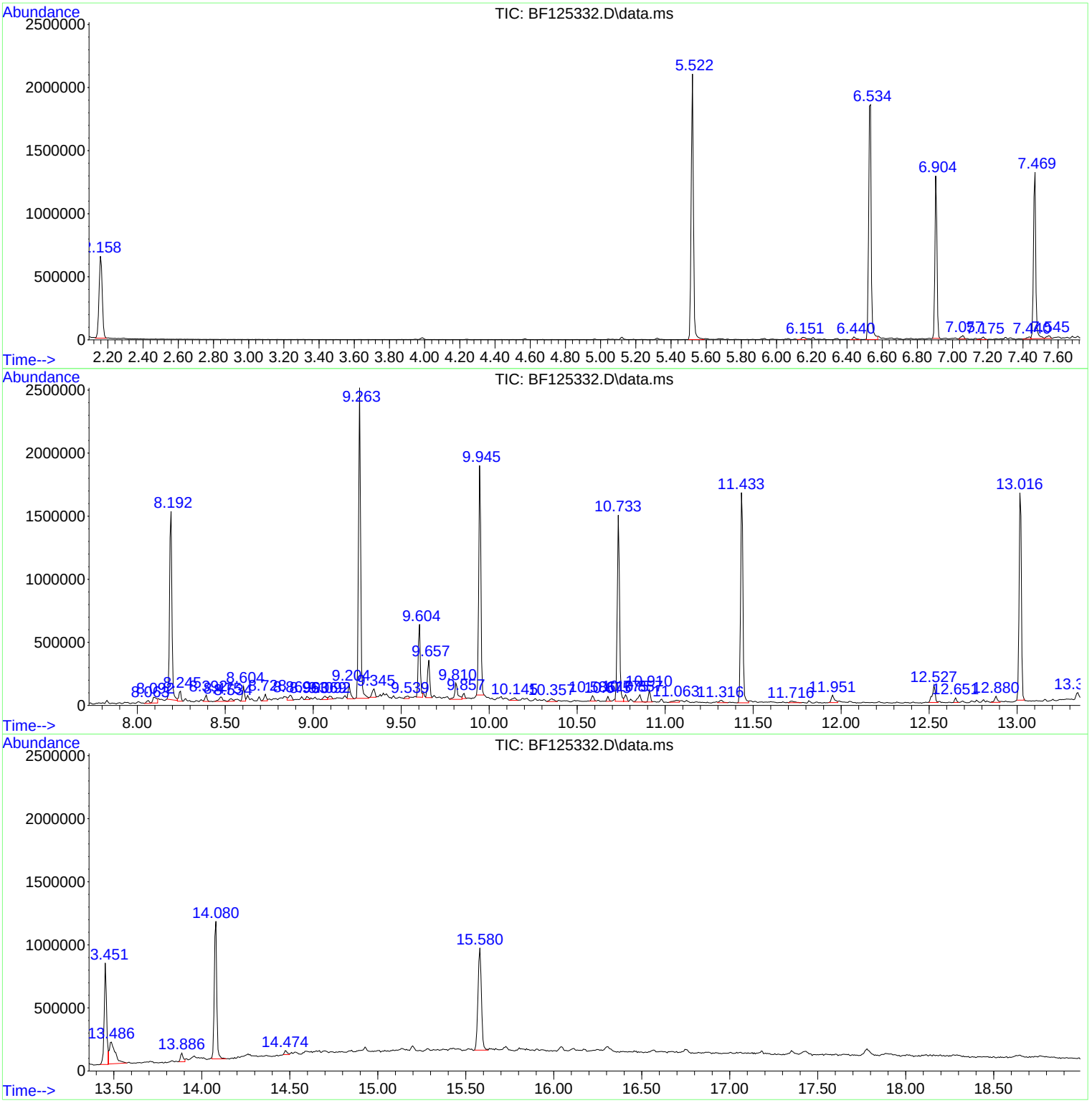
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
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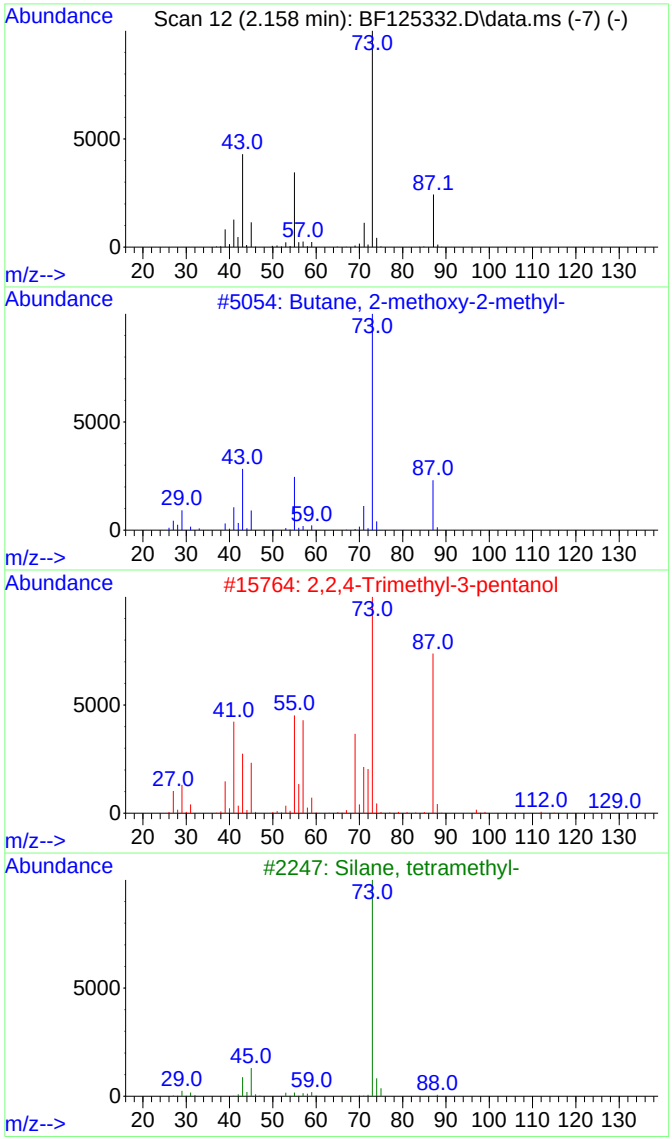
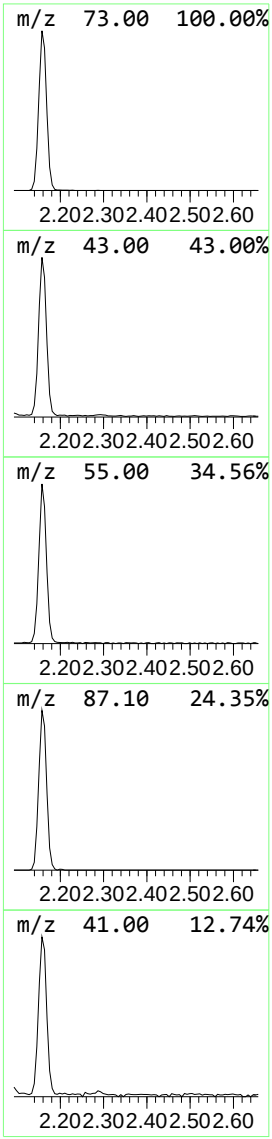
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	15.81 ng	818479	1,4-Dichlorobenzene-d4	6.904

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125332.D
Acq On : 2 Sep 2021 21:16
Operator : JU/CG
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-1

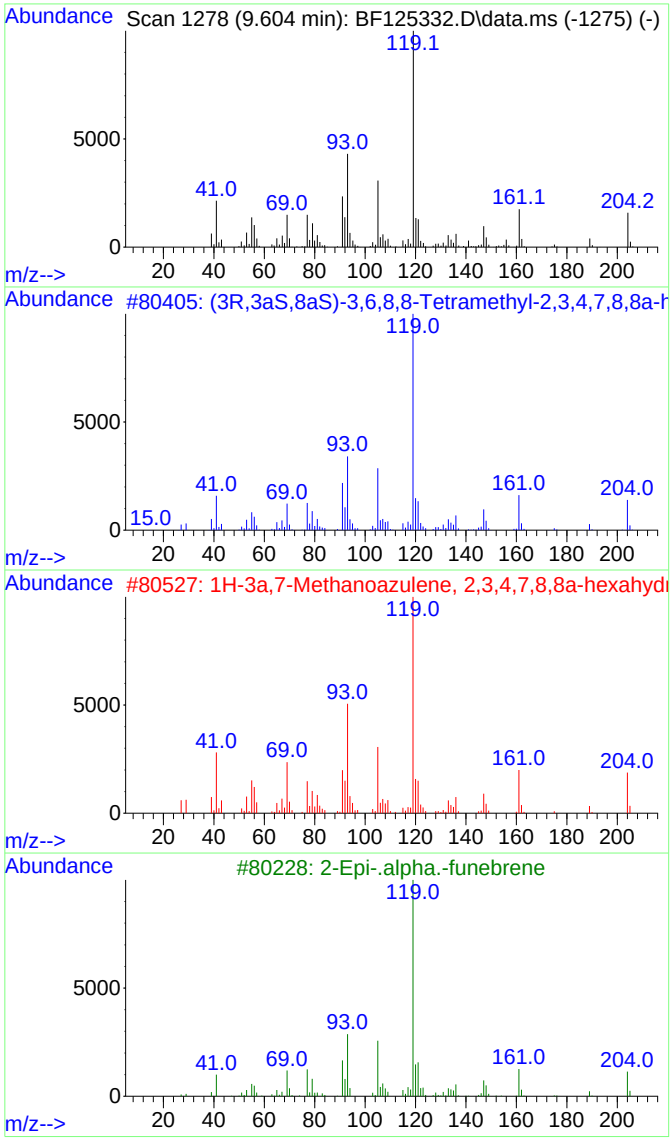
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

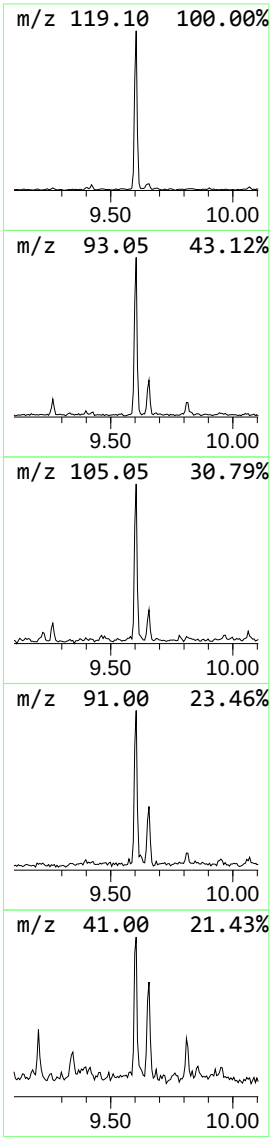
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (3R,3aS,8aS)-3,6,8,8-Tetram... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	6.31 ng	477892	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	98
2	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	97
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	93
4	(R)-1-Methyl-4-(6-methylhept-5-e...	204	C15H24	028976-67-2	86
5	1,3-Cyclohexadiene, 5-(1,5-dimet...	204	C15H24	000495-60-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125332.D
Acq On : 2 Sep 2021 21:16
Operator : JU/CG
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-1

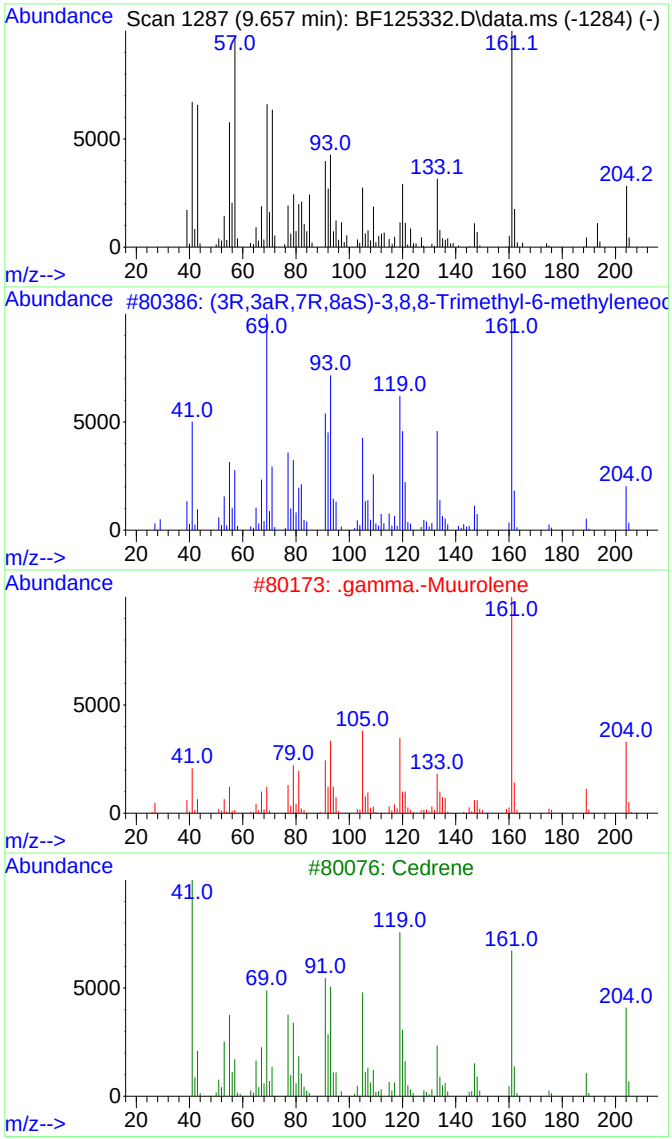
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

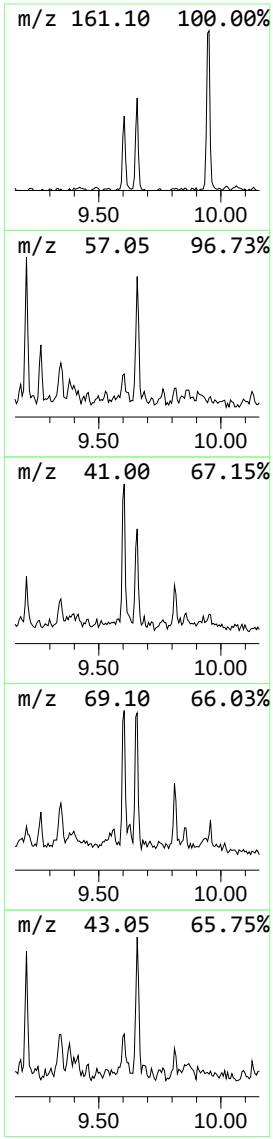
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (3R,3aR,7R,8aS)-3,8,8-Trime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	3.48 ng	263469	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3R,3aR,7R,8aS)-3,8,8-Trimethyl-...	204	C15H24	079120-98-2	93
2	.gamma.-Muurolene	204	C15H24	030021-74-0	58
3	Cedrene	204	C15H24	011028-42-5	55
4	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	52
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000546-28-1	50





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Instrument : BNA_F
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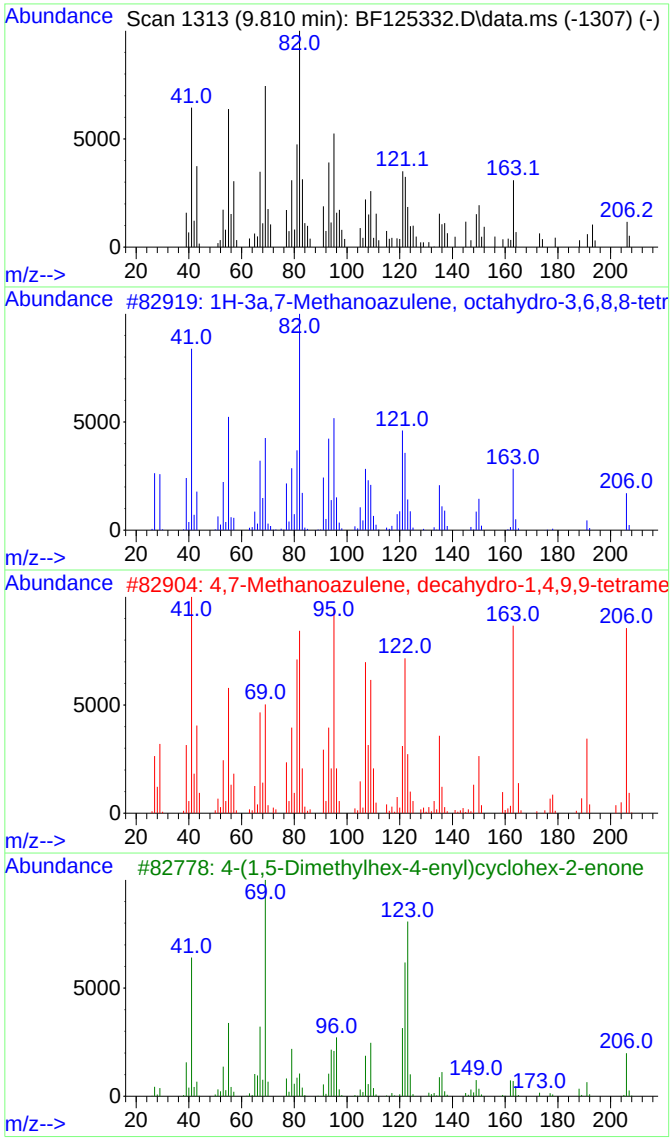
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

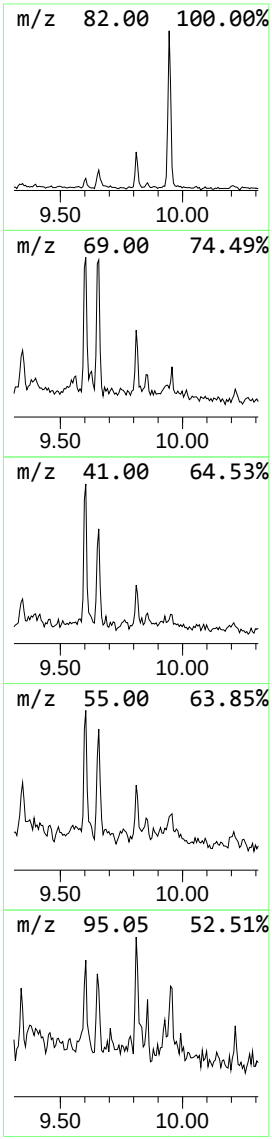
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-3a,7-Methanoazulene, oct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	2.10 ng	159370	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, octahydr...	206	C15H26	013567-54-9	92
2	4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	58
3	4-(1,5-Dimethylhex-4-enyl)cycloh...	206	C14H22O	001723-80-4	55
4	1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	38
5	1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	35





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Misc :
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Instrument : BNA_F
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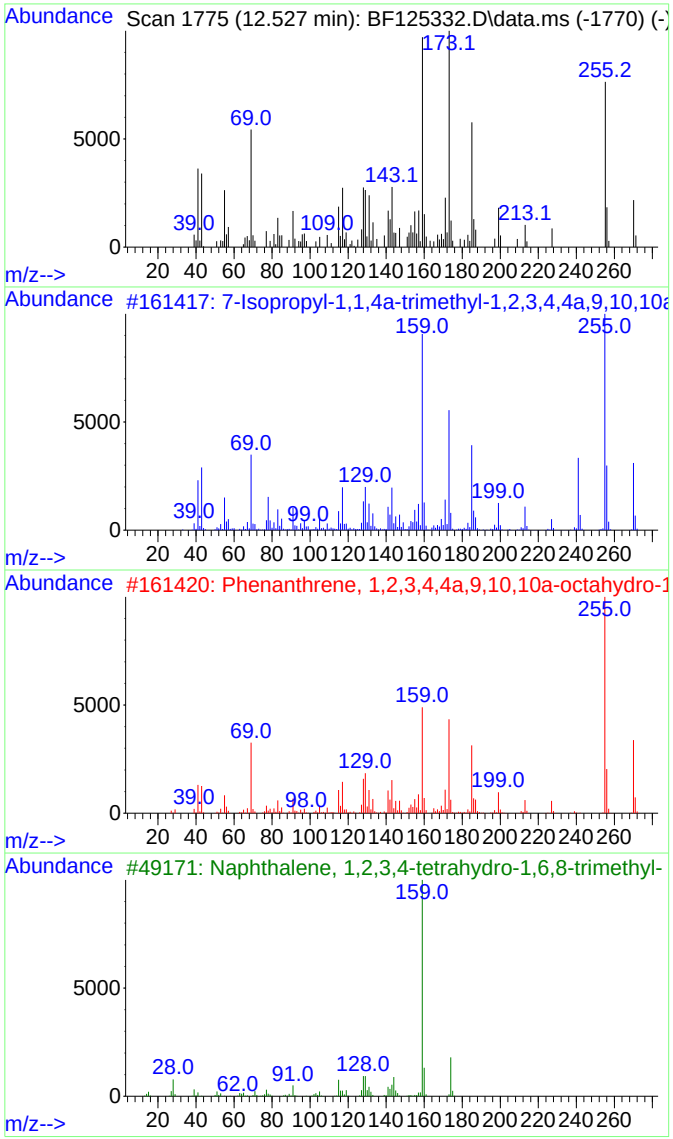
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

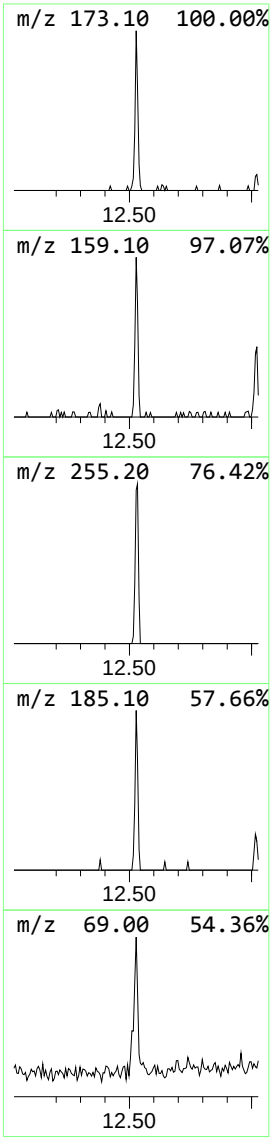
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 7-Isopropyl-1,1,4a-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	2.06 ng	157637	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Isopropyl-1,1,4a-trimethyl-1,2...	270	C20H30	109680-01-5	96
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	270	C20H30	019407-28-4	49
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	35
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	18
5	Iron, (.eta.-5-cyclohexadienyl)(...	270	C16H22Fe	1000162-99-3	15





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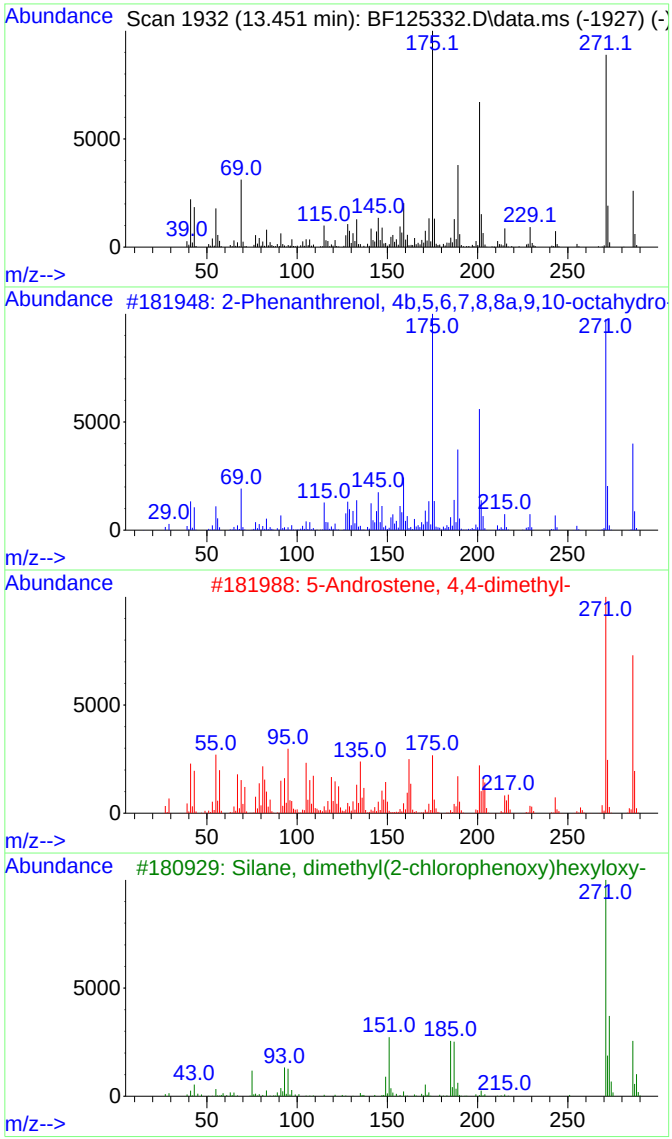
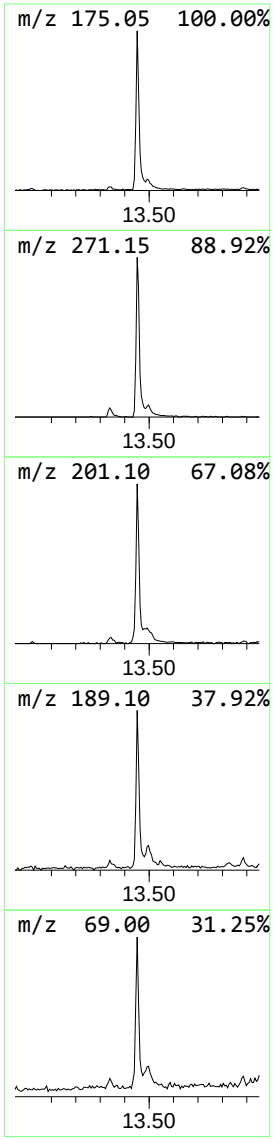
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	14.46 ng	771537	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	5-Androstene, 4,4-dimethyl-	286	C21H34	1000194-15-4	47
3	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-3	27
4	2-Methoxy-1-nitrophenazine 5,10-...	287	C13H9N3O5	023677-09-0	22
5	Benz(a)acridine, 9,10,12-trimethyl-	271	C20H17N	063040-02-8	18





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Sample : M3626-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : G-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

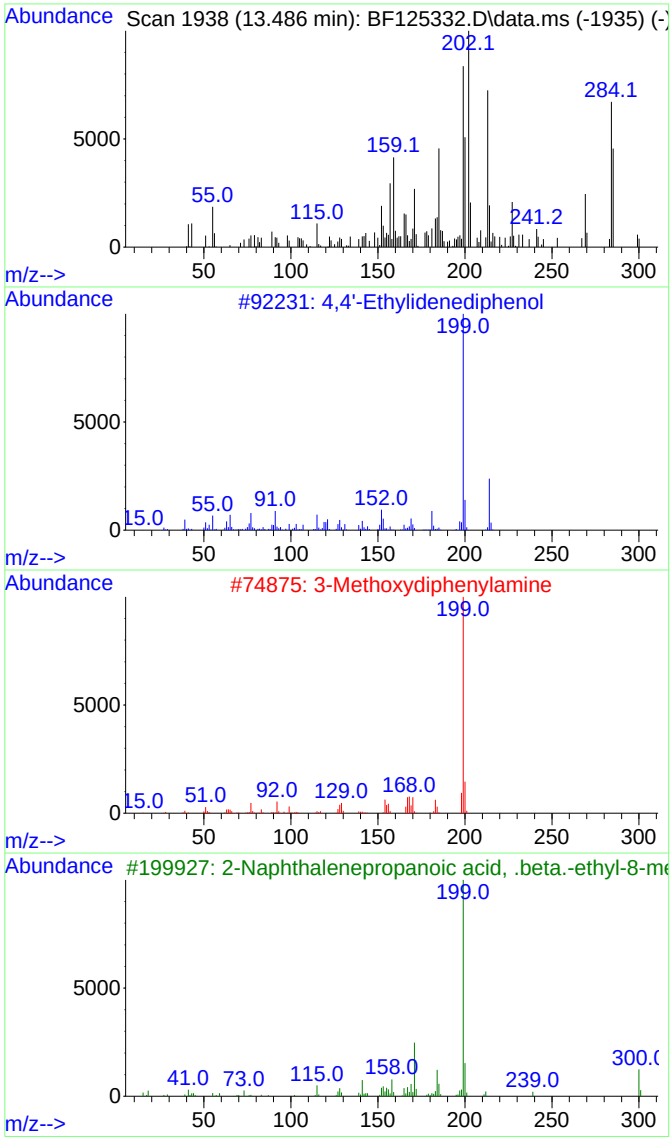
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

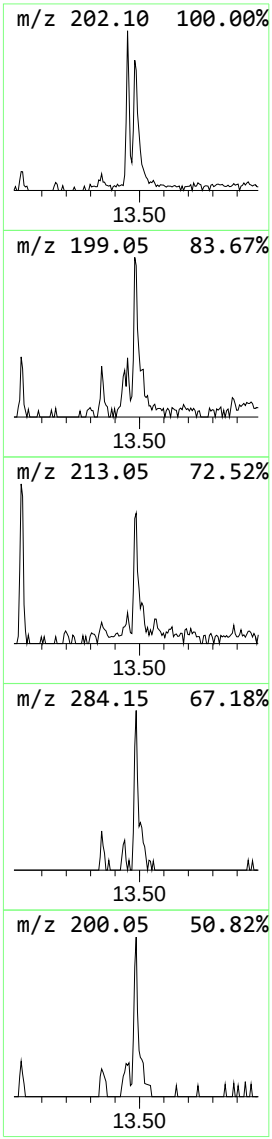
****

Peak Number 7 unknown13.486 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	7.20 ng	384220	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Ethylidenediphenol	214	C14H14O2	002081-08-5	15
2	3-Methoxydiphenylamine	199	C13H13NO	000101-16-6	15
3	2-Naphthalenepropanoic acid, .be...	300	C19H24O3	057289-69-7	15
4	1-tert-Butylpiperazine, TMS	214	C11H26N2Si	1000494-58-0	11
5	2-Ethylamino-3-piperidino-1,4-na...	284	C17H20N2O2	059641-39-3	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125332.D
Acq On : 2 Sep 2021 21:16
Operator : JU/CG
Sample : M3626-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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...	2.158	15.8	ng	818479	1	6.904	1035080	20.0
(3R,3aS,8aS)-3,...	9.604	6.3	ng	477892	3	9.945	1514720	20.0
(3R,3aR,7R,8aS)...	9.657	3.5	ng	263469	3	9.945	1514720	20.0
1H-3a,7-Methano...	9.810	2.1	ng	159370	3	9.945	1514720	20.0
7-Isopropyl-1,1...	12.527	2.1	ng	157637	4	11.433	1531990	20.0
2-Phenanthrenol...	13.451	14.5	ng	771537	5	14.080	1067350	20.0
unknown13.486	13.486	7.2	ng	384220	5	14.080	1067350	20.0